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ADVANCED STREAMING AGENT DEVELOPMENT (PHASE IIA): MEDIUM-SCALE TESTING OF ADVANCED AGENT COMPOUNDS

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14. ABSTRACT

This project is an investigation of advanced fire suppression agents as replacements for Halon 1211 used in U.S. Air Force flightline and aircraft portable fire extinguishers. Materials tested in this test series emphasized agent blends containing bromoalkanes. Baseline tests were run with Halon 1211. The testing took into account agent discharge patterns, flow rates, wind conditions and technique, and allowed comparison of agent effectiveness to that of Halon 1211. Blends of small amounts (up to 24 weight percent) of 1-bromopropane in a hydrofluoropolyether showed enhanced fire extinguishment performance over that of either of the pure components. Similar enhancement was seen with HFC-23fa and 1-bromopropane. Results were compared to those obtained in similar testing performed for the U.S. Army.

15. SUBJECT TERMS

bromoalkanes, fire suppression agents, halon, Halon 1211, streaming agents, halon replacements, 1-bromopropane

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PREFACE

This report was prepared by the Center for Global Environmental Technologies (CGET) Division, New Mexico Engineering Research Institute (NMERI), The University of New Mexico, Albuquerque, New Mexico, for the Infrastructure Technology Section of Wright Laboratory (WL/FIVCF), Tyndall Air Force Base, Florida, and Applied Research Associates (ARA), Inc., Tyndall Air Force Base, Florida, under SETA Task 3.12, Air Force Contract S-5000.38, NMERI Number 8-32760.

The Start Date was 29 April 1996, and the End Date was 28 February 1997. The WL/FIVCF Project Officer was Major Robert A. Tetla, the ARA Project Officer was Michael A. Rochefort, and the NMERI Principal Investigator was Robert E. Tapscott.

The objective of the overall effort is to develop new chemical compounds that are highly efficient fire suppressants, have low environmental and toxicological impacts, have the same performance characteristics as Halon 1211 (bromochlorodifluoromethane, BCFC-12B1, $CBrClF_2$) and are compatible with existing fire extinguishing equipment and aircraft materials. This report covers the Phase IIA initiation of medium-scale field testing.

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EXECUTIVE SUMMARY

A. OBJECTIVE

The objective of the overall effort is to develop new chemical compounds that are highly efficient fire suppressants, have low environmental and toxicological impacts, have the same performance characteristics as Halon 1211 fire extinguishant, and are compatible with existing fire extinguishing equipment and aircraft materials. The effort includes syntheses of new compounds, laboratory analyses of fire suppression characteristics, analyses of environmental and toxicity parameters, and analyses of stability, compatibility, and manufacturability factors. The goal of the present effort is the initiation of medium-scale field fire extinguishment testing.

B. BACKGROUND

Under the Montreal Protocol, an international treaty enacted in 1987 and amended in 1990, 1992, and 1995, the production of the fire and explosion protection agents Halon 1211, Halon 1301, and Halon 2402 was phased out in the United States at the end of 1993. To date, no environmentally acceptable halon substitute that is equivalent to the existing halons in toxicity, effectiveness, cleanliness, and dimensionality has been identified.

Halocarbons as replacements for halons have been well studied, and it is unlikely that new, exceptionally effective, halon replacements will be identified among the normal saturated halocarbons (excluding iodides and other halocarbons with chemical features leading to short atmospheric lifetimes). Thus, materials other than the normal saturated halocarbons are being investigated. These "advanced agent" materials include non-halocarbons and halocarbons with chemical features leading to very short atmospheric lifetimes ("tropodegradable" halocarbons).

In Phase IA of this program, several potential advanced agent substitutes for halons were identified and underwent preliminary screening and testing. In Phase IB, these materials underwent further evaluation to complete the selection of materials to proceed to Phase II, medium-scale and large-scale field testing. The present report covers the Phase IIA initiation of medium-scale fire suppression testing.

C. SCOPE

This project is an investigation of advanced fire suppression agents to find a replacement for Halon 1211 fire extinguishant used in Air Force flightline and aircraft portable fire extinguishers. The overall project builds on prior Air Force research and concentrates primarily on phosphorus compounds (with an emphasis on phosphorus nitrides), metal-containing compounds, silicon derivatives, and tropodegradable halocarbons. Other families with equal or better probability of success, which come to light during this contract period, are to be included in the investigation.

Phase IIA consists of two tasks (the numbering follows from that given in the Phase IB Statement of Work):

Task 5: Medium-Scale Testing of Advanced Agent Compounds. The extinguishing performance of those advanced agent compounds selected as most promising in Phase IB in extinguishing fires will be assessed using medium-scale streaming tests.

Task 6: Final Report. The information obtained will be used to prepare a final report detailing the work performed, the results obtained, and conclusions. The report is to make recommendations for continuation of the medium-scale testing, as well as large-scale testing, with the most promising agents.

D. METHODOLOGY

Researchers typically rely on laboratory-scale cup-burner test results as an indicator of fire extinguishing effectiveness of volatile (gaseous) agents, those of primary interest as Halon 1211 substitutes. In general, agent performance in a total-flood application improves with decreasing cup-burner extinguishing concentrations. This, however, is not always true in streaming applications. The evaluation of agent effectiveness in streaming applications at larger scale can be complex. Any move from laboratory-scale testing to medium-scale field testing for streaming introduces a new set of variables that must be understood and controlled. Discharge pattern, flow rate, wind conditions, and technique can have a significant impact on agent

performance. If these variables are not considered and controlled, they can have a compounding effect, causing test results to be invalid, or worse yet, misleading.

The move from laboratory to field-scale testing also introduces a new problem—agent consumption. A single medium-scale field test can require over 50 times more agent than a laboratory test. Since agent quantities are usually limited, care must be taken to ensure tests are performed carefully so that optimum information can be gained from each test.

Prior to initiating the research reported here, a careful analysis was made of all factors affecting agent performance in streaming applications. Test conditions and techniques were developed to address variables affecting performance, and a final test design was developed to optimize testing.

E. APPROACH

A test approach providing optimal information with minimal agent use was developed and used. Tests were conducted with 18-in x 18-in (45.7-cm x 45.7-cm) x 6-in (15.24-cm) deep square pans having a surface area of 2.25-ft^2 (0.209-m^2). Heptane was used as the fuel. Tests were run with a constant flow rate extinguisher to eliminate variability resulting from fill ratio. Blends of bromoalkanes with non-brominated halocarbons were a major emphasis of this Phase IIA work. Non-brominated halocarbon components were evaluated based on their boiling points and other physical properties, and two were chosen to be tested at field scale—HFC-236fa (1,1,3,3,3-hexafluoropropane, $CF_3CH_2CF_3$) and a hydrofluoropolyether (HFPE-1164X). These agents were blended with bromoalkanes, including 1-bromopropane and 1-bromobutane. Baseline tests were also run with Halon 1211 and perfluorohexane ($CF_3CF_2CF_2CF_2CF_2CF_3$), a halocarbon with a relatively high boiling point that exhibits performance similar to that of the HFPE-1164X in laboratory-scale extinguishment "streaming" experiments. A cyclotriphosphazene fluid, $[P_3N_3(OCH_2CF_3)_{3.5}(OC_6H_5)_{1.25}(m\text{-}OC_6H_4CH_3)_{0.87}\text{-}(p\text{-}OC_6H_4CH_3)_{0.37}]$, was also tested.

F. RESULTS

Extinguishment results were obtained with two bromoalkanes, 1-bromopropane ($CH_3CH_2CH_2Br$) and 1-bromobutane ($CH_3CH_2CH_2CH_2Br$) and carriers including HFPE-1164X and HFC-236fa. Perfluorohexane and the cyclotriphosphazene fluid were also tested. The results indicate the following:

1. Neat (i.e., nonblended) HFPE-1164X appears less effective than C_6F_{14}, although the HCFC does extinguish fires.

2. Neat 1-Bromopropane is not highly effective in extinguishing fires as a pure agent; however, blending with a nonflammable carrier provides a marked improvement in performance.

3. Blends of HFPE-1164X with 1-bromopropane were more effective in extinguishing fires than either components alone. The lowest obtainable flow rate that resulted in extinguishment of 2.25-ft^2 (0.209-m^2) heptane fires with neat HFPE-1164X was 0.38 lb/s (0.17 kg/s). The addition of 25 wt.% 1-bromopropane, gave extinguishment at a flow rate of 0.29 lb/s (0.13 kg/s). The addition of 10 wt.% 1-bromopropane to HFPE-1164X gave a blend with an extinguishment flow rate of 0.17 lb/s (0.077 kg/s), an even better performance.

4. A significant enhancement compared to the neat carrier was also seen with the addition of 1-bromopropane to HFC-236fa. With 10 wt.%, 15 wt.%, and 25 wt.% 1-bromopropane blends, extinguishment quantities for 2.25-ft^2 (0.209-m^2) heptane fires ranged from 0.7 to 1.1 pounds (0.3 to 0.50 kilograms), compared to 1.7 to 2.6 pounds (0.77 to 1.2 kilograms) for neat HFC-236fa. The associated flow rates ranged from 0.15 to 0.22 lb/s (0.068 to 0.10 kg/s) for both the pure chemical and the blends. Overall, the 1-bromopropane reduced the extinguishment quantities of the HFC-236fa by more than 50 percent. A similar enhancement was seen with a 15 wt.% blend of 1-bromobutane with HFC-236fa.

5. The cyclotriphosphazene fluid was not effective in extinguishing 2.25-ft^2 (0.209-m^2) heptane fires, either blended or by itself. The fluid was very viscous, and the spray pattern was tight and not well-dispersed.

G. CONCLUSIONS

Blends of bromoalkanes (especially 1-bromopropane) with HFC-236fa and HFPE-1164X show enhanced suppression capability over that of pure HFC-236fa and HFPE-1164X. This enhancement was significant on 2.25-ft^2 (0.209-m^2) heptane fires, reducing the agent required for extinguishment by as much as 50 percent at similar flow rates. Tests performed for the U.S. Army under a separate contract, utilizing HFC-227ea, HFC-236fa, and HFPE-1164X blended with 1-bromopropane and tested on 5- and 12.5-ft^2 (2.32- and 1.16-m^2) Jet-A fuel fires, showed similar enhancement.

H. RECOMMENDATIONS

Tests should be performed with bromoalkane blends (in particular, 1-bromopropane blended with HFC-236fa and HFPE-1164X) on larger-scale heptane and Jet-A fires, including 12.5-ft^2 (1.16 m^2) (Underwriters Laboratories (UL)-5B) and 25-ft^2 (2.32 m^2) (UL-10B) fires. UL-approved halon-type extinguishers should be used, and comparisons should made with currently available halon replacements. It is important that proper nozzles, fill densities, and nitrogen pressures be used to obtain optimum performance.

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LIST OF ABBREVIATIONS

ARA	Applied Research Associates
ALC	Approximate Lethal Concentration
BCFC	bromochlorofluorocarbon
BFC	bromofluorocarbon
CAS	Chemical Abstracts Service (American Chemical Society)
CCOD	CGET Chemical Options Database
CGET	Center for Global Environmental Technologies
FC	(per)fluorocarbon
GWP	Global Warming Potential
HBC	hydrobromocarbon
HCFC	hydrochlorofluorocarbon
HFC	hydrofluorocarbon
HFPE	hydrofluoropolyether
LC_{LO}	lowest concentration causing death
LC_{50}	concentration required to cause death in 50 percent of an animal test population
LOAEL	Lowest Observed Adverse Effect Level
LSDE	Laboratory-Scale Discharge Extinguishment
NMERI	New Mexico Engineering Research Institute
NOAEL	No Observed Adverse Effect Level
ODP	Ozone Depletion Potential
PFC	perfluorocarbon
SCBA	Self-contained Breathing Apparatus
SVEq	storage volume equivalent
TACOM	Tank-Automotive and Armament Command
UL	Underwriters Laboratories, Inc.
USAF	United States Air Force
WEq	weight equivalent

LIST OF UNITS AND SYMBOLS

A	nozzle cross-sectional area
C	discharge coefficient
C_c	coefficient of continuity
C_V	coefficient of velocity
°C	degrees Celsius
cm	centimeter
°F	degrees Fahrenheit
ft	foot
g	gram
g	gravitational constant, and
h	pressure head
gal	gallon
in	inch
kg/s	kilogram/second
kPa	kilopascal
L	liters
lb	pound
lb_f/in^2	pounds force per square inch
lb_f/ft^2	pounds force per square foot
lb/s	pound per second
$lb/sec\text{-}ft^2$	pound per second per square foot
m	meter
mL	milliliters
P	fluid pressure at the nozzle inlet
Q	flow in volume per second
N_R	Reynolds Number
s	second
t	time

LIST OF UNITS AND SYMBOLS (CONCLUDED)

v	fluid velocity of exit from the nozzle
vol.%	percent by volume
wt.%	percent by weight
ρ	fluid density
μ	micron
μ	fluid viscosity
ν	dynamic viscosity.

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SECTION I
INTRODUCTION

A. OBJECTIVE

The objective of the overall effort is to develop new chemical compounds that are highly efficient fire suppressants, have low environmental and toxicological impacts, have the same performance characteristics as Halon 1211 (bromochlorodifluoromethane, $CBrClF_2$, BCFC-12B1, CAS Number 353-59-3, CCOD ID 151) and are compatible with existing fire extinguishing equipment and aircraft materials.* The effort includes syntheses of new compounds; laboratory analyses of fire suppression characteristics; analyses of environmental and toxicity parameters; analyses of stability, compatibility, and manufacturability factors; and medium-scale field testing. This report covers only the medium-scale field tests (Phase IIA). The remaining studies are reported in the Phase IB report (Reference 1).

B. BACKGROUND

Under the Montreal Protocol, an international treaty enacted in 1987 and amended in 1990, 1992, and 1995, the production of the fire and explosion protection agents Halon 1211, Halon 1301 (bromotrifluoromethane, $CBrF_3$, BFC-13B1, CAS Number 75-63-8, CCOD ID 503), and Halon 2402 (1,2-dibromo-1,1,2,2-tetrafluoroethane, $CBrF_2CBrF_2$, BFC-114B2, CAS Number 124-73-2, CCOD ID 27) was phased out in the United States at the end of 1993.† To date, no environmentally acceptable halon substitute that is equivalent to the existing halons in toxicity, effectiveness, cleanliness, and dimensionality has been identified.

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* Here, and elsewhere in this report, the halocarbon number (e.g., BCFC-12B1) is given. Since there is no widely available source describing the derivation of these Halocarbon Numbers, an up to date overview is given in Appendix A. The CAS number is a designation assigned by the Chemical Abstracts Service of the American Chemical Society. Since not all compounds have had CAS numbers assigned, ID numbers from the CGET Chemical Options Database (CCOD) are also given for chemicals discussed in this report. The Chemical Options Database is an expanded version of a database prepared under U. S. Environmental Protection Agency (EPA) sponsorship and provides a unique ID number for each compound (Heinonen, E. W., and Tapscott, R. E., *CGET/EPA Chemical Options Database User's Manual*, ICF Incorporated, Washington, DC, December 1995).

† Only Halon 1211 and Halon 1301 have had significant use in the United States. The primary use of Halon 2402 has been in the Former Soviet Union and in a few eastern European countries.

Halocarbons as replacements for halons have been well studied, and it is unlikely that new, exceptionally effective, halon replacements will be identified among the fluorine-containing saturated halocarbons, which have been the primary focus in past efforts. The hydrochlorofluorocarbons (HCFC), perfluorocarbons (PFC or FC), and hydrofluorocarbons (HFC) are all less effective than the present halons in most scenarios. Moreover, all of these have some adverse global environmental impact (ozone depletion, global warming, and/or long atmospheric lifetime). PFCs and HCFCs are already subject to some restrictions, and such restrictions may eventually extend to HFCs (Reference 2). The single partial success among halocarbon replacements are fluorioiodocarbons, in particular, trifluoromethyl iodide (CF_3I, IFC-13I1, CAS Number 2314-97-8, CCOD ID 100), which is as effective as the existing halons. However, the toxicity of the iodides mandates that their use be restricted to only certain applications. There is, therefore, an increasing reason to look at compounds other than the normal saturated halocarbons—non-halocarbons and halocarbons with chemical features leading to very short atmospheric lifetimes ("tropodegradable" halocarbons). These compounds are collectively designated "advanced agents" (Reference 3).

In Phase IA of this program, several potential advanced agent substitutes for halons were identified and underwent preliminary screening and testing. Tropodegradable halocarbons (e.g., alkenes, aromatics, polar-substituted halocarbons) were identified as highly promising candidates for halon replacement (Reference 4). The most promising of the non-halocarbon agents were found to be phosphorus compounds, particularly the phosphorus nitrides (Reference 5); metal compounds (Reference 6); and silicon derivatives (Reference 7).

In Phase IB, these materials underwent further evaluation to complete the selection of materials to proceed to Phase II, medium-scale and large-scale field testing. The Phase IB evaluation included such items as (1) assessment of syntheses and manufacturability, (2) toxicicity review, and (3) decomposition product analysis (Reference 1). During the Phase IB testing, it became increasingly apparent that bromoalkane blends and tropodegradable halocarbons held particular promise as streaming agents. As a result, the project began to focus on such blends and on tropodegradable halocarbons with a decreased emphasis on non-halocarbon materials. The present report covers the Phase IIA initiation of medium-scale testing

for evaluating some of these materials as fire extinguishing agents for United States Air Force (USAF) streaming applications.

C. SCOPE

The overall project is an investigation of advanced fire suppression agents to find a replacement for Halon 1211 used in USAF flightline and aircraft portable fire extinguishers. The research builds on prior USAF research and concentrates primarily on tropodegradable halocarbons and non-halocarbons (phosphorus nitrides, metal compounds, and silicon compounds). Other families with equal or better probability of success, which come to light during this contract period, were, however, to be included in the investigation. Blends of bromoalkanes, which are tropodegradable halocarbons, were found to have a high probability of success, and, for this reason, a significant amount of the investigation has been on these materials. The present Phase IIA report covers the medium-scale field testing with an emphasis on bromoalkane blends. Additional work on other tropodegradable halocarbons with an emphasis on non-blended ("neat") agents is anticipated.

Phase IIA consists of two tasks, 5 and 6. (Results for Tasks 1 through 4 (Phase IB) are reported in Reference 1.)

Task 5: Medium-Scale Testing of Advanced Agent Compounds. The extinguishing performance of those advanced agent compounds selected as most promising in Phase IB in extinguishing fires is to be assessed using medium-scale streaming tests.

Task 6: Final Report. The information obtained is to be used to prepare a final report detailing the work performed, the results obtained, and conclusions. The report is to make recommendations for continuation of the medium and large-scale testing with the most promising agents.

D. METHODOLOGY

Laboratory-scale cup-burner test results are often used as an indicator of agent fire extinguishing effectiveness. Agents with low cup-burner extinguishment concentrations usually

perform well in total-flood applications. This is not always true for streaming applications, where the agent streaming characteristics have an important, though complex, effect on performance. The move from laboratory-scale testing to field testing introduces a whole new set of variables that must be understood and controlled. The effect of agent discharge patterns, flow rates, wind conditions, and technique can have a significant impact on agent performance. If these variables are not considered and controlled, they can have a compounding effect, causing test results to be invalid or misleading.

The move from laboratory to field-scale testing also introduces the problem of agent consumption. A single medium-scale field test can require more than 50 times the agent needed for a laboratory test. Since agent quantities are usually limited, care must be taken to ensure tests are performed carefully so that optimum information can be gained from each test. For these reasons, a significant part of this Phase IIA test program emphasized development and assessment of the test procedures and result analyses.

E. APPROACH

Laboratory-scale testing indicates hydrobromocarbon (HBC) blends show particular promise as halon replacements (Reference 1). Such blends are a mixture of a bromine-containing component, which provides a chemical fire extinguishment mechanism, and a non-bromine containing component, which modifies the streaming performance, lowers the fire temperature by heat absorption to enhance the efficacy of the bromine-containing component, and may provide additional benefits (e.g., lowered cost, improved environmental characteristics, elimination of agent flammability, and decreased toxicity). For simplicity, these non-bromocarbon components are termed "carriers." Note, however, that the term "carrier" is not meant to imply that the non-bromocarbon component has no intrinsic involvement in fire extinguishment.

An approach to testing agents to provide optimal information with minimal agent use was developed and used. The same firefighter was used in all tests conducted during this phase of the project. Firefighter technique is considered the single most significant variable, and it was critical to use a single firefighter to allow a direct comparison between agents.

Another variable of concern was wind conditions. All testing was performed at a site that maintained outdoor test conditions, yet protected the fire from light winds. Winds above 5 miles per hour, or swirling winds, were not acceptable. Winds can make a fire easier or harder to extinguish, depending on the wind direction. If satisfactory test conditions were not met, testing was not performed.

During this phase of work, several compounds and compound blends were tested using the procedures described in Section E. Streaming test data developed for the U. S Army are also shared in this report with U. S. Army permission.

SECTION II

TEST SETUP

A. TEST SITE

The tests were performed at the New Mexico Engineering Research Institute (NMERI) test site located in Albuquerque, New Mexico. The test site (Figure 1) is located in a non-populated area and is approximately 0.5 mile (0.81 kilometer) away from any occupied buildings. The tests were conducted on a concrete test pad surrounded by a circular metal enclosure with a diameter of approximately 50 feet (15.2 meters), a height of approximately 12 feet (3.7 meters), and open at the top. The enclosure (wind break) protected the test pans from light winds, yet maintained outside test conditions allowing sufficient air for the combustion process. The pans were placed far enough from the edge of the wind break to avoid any agent reflection back onto the pan. The emissions and operations associated with the NMERI test site comply with current local, state, and national environmental and safety regulations.

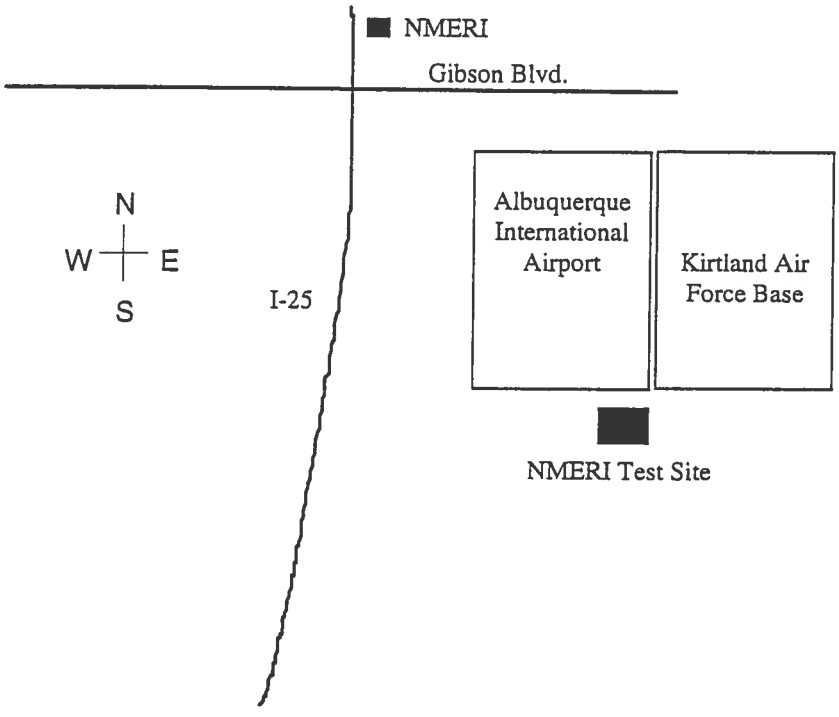

Figure 1. Test Site Location.

B. FIRE PANS

Tests were conducted with 18-in x 18-in (45.7-cm x 45.7-cm) x 6-in (15.24-cm) deep square pans having a surface area of 2.25-ft^2 (0.209-m^2). Heptane was floated on 2 inches (5.1 centimeters) of water, leaving a 2-in (5.1-cm) freeboard. Two fire pans were typically alternated during each test series, preventing excessive overheating of the fuel and fire pan and increasing the number of tests conducted in a day.

C. ASSOCIATED TEST EQUIPMENT

Various equipment and supplies were required to perform the tests. Table 1 lists the materials and associated functions.

TABLE 1. MEDIUM-SCALE TEST EQUIPMENT AND SUPPLIES.

Item	Function
Nitrogen cylinders and hardware	Extinguisher pressurization
Heptane	Fuel
Approved containers	Transporting, pouring, and storing fuel
Propane torch	Fuel ignition
Scale	Weigh fire extinguishers
Firefighter equipment such as self-contained breathing apparatus (SCBA), fire suits, fire helmets, boots, etc.	Firefighter protection
Stopwatch	Monitoring preburn and extinguishment times
Video cameras/tapes	Test documentation
Megaphone	Test direction
Back-up dry chemical fire extinguishers	Fire extinguishment
Cellular phone	Emergency use
Test agents	

D. EXTINGUISHER

The NMERI 1-Gallon (3.79-liter) Constant-Flow Rate Extinguisher (Figure 2), which eliminates variability due to fill ratio change, was used for the testing. The extinguisher is comprised of a stainless steel cylinder, having a valve assembly on top for filling and pressurization, and a hose leading to the nozzle assembly on the bottom. A nitrogen line providing a constant pressure is connected to the top, ensuring a constant flow. Standard Amerex halon nozzles, with different diameter bores, were attached to the nozzle assembly.

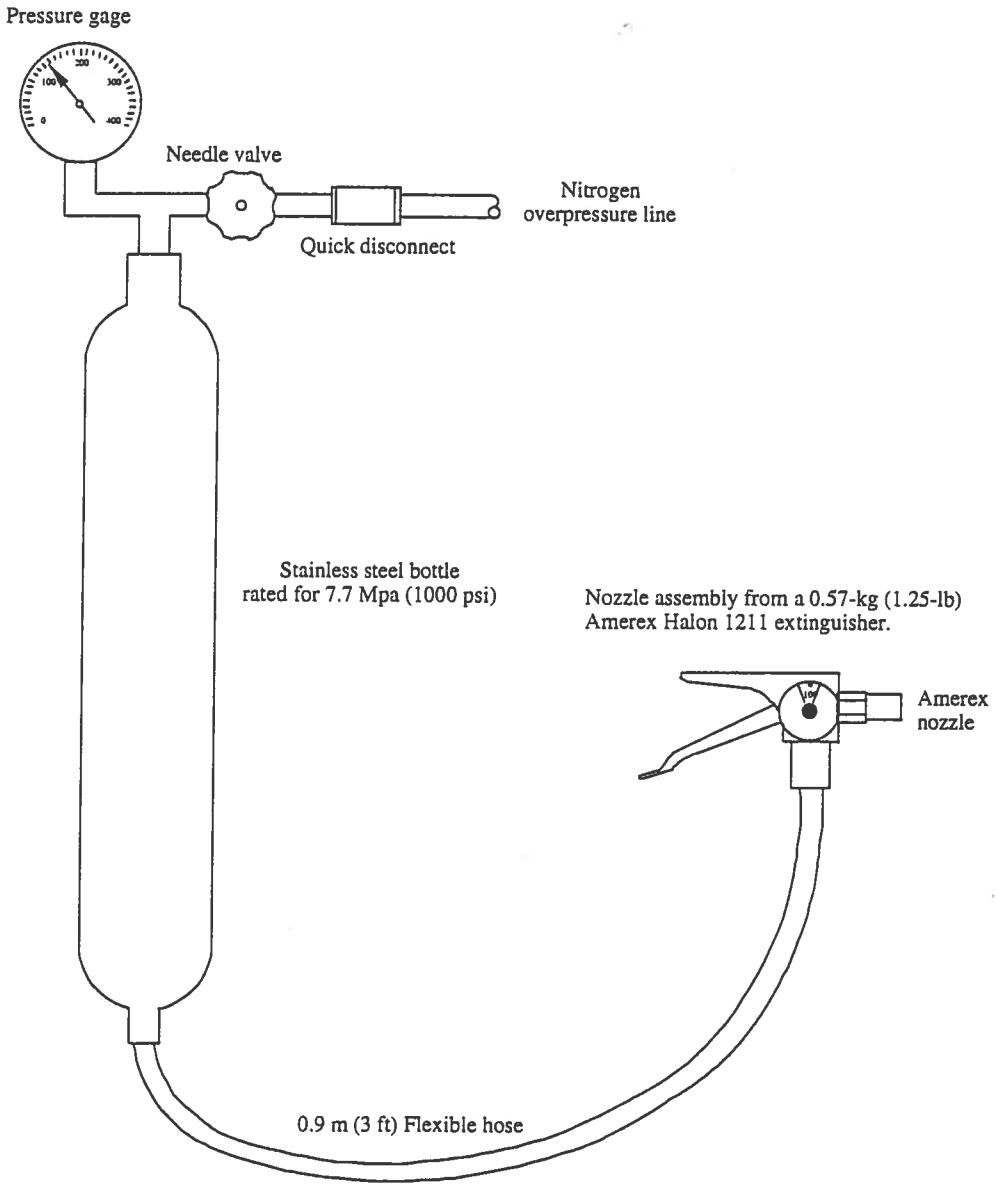

Figure 2. NMERI 1-Gallon (3.79-liter) Constant-Flow Rate Extinguisher.

E. TEST PROCEDURES

Testing reported here uses 2.25-ft^2 (0.209-m^2) heptane fires. The agent is loaded into the NMERI 1-Gallon (3.79-liter) Constant-Flow Rate Extinguisher, charged with nitrogen, shaken to ensure saturation of the nitrogen, and after a 60-second preburn, applied to the front edge of the flame, at its base, in a side-to-side sweeping motion (approximately 2 sweeps/second). The flame front is pushed to the back of the pan while the firefighter maintains the sweeping motion. The fire is held there until it is extinguished. The fire is attacked at an angle of approximately 30 to 45 degrees from vertical. The extinguishment time is determined with a stopwatch. After extinguishment, the extinguisher is weighed to determine the amount of agent used. The flow rate is determined by dividing the weight of agent discharged by the extinguishment time. By knowing the weight of agent discharged, the extinguishment time, and the flow rate, agents can be compared to determine their relative effectiveness.

SECTION III
BROMOALKANE BLENDS

A. OVERVIEW

During Phase IB of this project, it was found that bromoalkanes, when blended with a carrier, exhibit enhancement of extinguishing performance in cup-burner and laboratory-scale discharge extinguishment (LSDE) tests compared to the performance of the carrier alone (Reference 1). For flammable bromoalkanes, the carrier was nonflammable or had a low flammability.

B. CARRIER SELECTION

The selection targets for carriers in the bromoalkane blends are presented Table 2. A review of the NMERI Chemical Options Database (Reference 8) was performed to develop a list of potential carriers (Table 3). The GWP (Global Warming Potential) is the change in radiative forcing resulting from the emission of 1 kilogram of a chemical relative to the radiative forcing resulting from the emission of 1 kilogram of a reference gas. The time period used to calculate the GWP is termed the "time horizon" (Reference 4). The LC_{50} and ALC values are measures of the acute toxicity of a compound. The LC_{50} is the concentration required to cause death in 50 percent of an animal test population. All LC_{50} values given in Table 3 are for 4-hour rat exposures. The ALC (Approximate Lethal Concentration) approximates the lowest concentration that causes death (LC_{LO}). Thus, it is lower than the LC_{50} value. The ALC value is often used in place of the LC_{50} in assessing safety. The values in the table are LC_{50} values unless otherwise noted. The NOAEL (No Observed Adverse Effect Level) is the highest exposure level that has been observed to cause no adverse effect; the LOAEL (Lowest Observed Adverse Effect Level) is the lowest exposure level that has been observed to cause an adverse effect. For all of the compounds in Table 3, the adverse effect on which the NOAEL and LOAEL values are based is cardiac arrhythmias as induced in dogs by inhalation. The WEq (Weight Equivalent) and SVEq (Storage Volume Equivalent) values give the calculated weight or storage volume relative

TABLE 2. CRITERIA FOR IDEAL CARRIERS.

Criteria	Value
ODP	Zero
Atmospheric Lifetime	< 50 yrs
GWP	< 10,000
Availability	Currently or in the very near future being manufactured or investigated for various uses.
Effectiveness	WEq < 3.0
Boiling Point	< 100 °C
Toxicity	LC_{50} > 18 volume percent
Cost	< $50 per lb

to Halon 1211 based on the cup burner extinguishment concentrations. The method for calculating these values is given in Reference 2.

Three carriers were selected for consideration, a low, intermediate, and high boiling point compound: HFC-227ea (boiling point -16.4 °C, 2.5 °F), HFC-236fa (boiling point -1.4 °C, 29.5 °F), and HFPE-1164X* (boiling point 100 °C, 212 °F). All three of the carriers are now available at a reasonable cost. Testing of compounds within these boiling point ranges allows a determination of the effect of carrier volatility on bromoalkane blend performance. Two of these compounds —HFC-236fa and HFPE-1164X—were selected to be tested in this USAF work.

* The hydrofluoropolyether (HFPE) H-Galden 1164X was supplied as an experimental sample by Ausimont S.p.A., Bollate (Milano), Italy and has an average molecular weight of 325 and a formula $HF_2CO(CF_2O)_n(CF_2CF_2O)_m CF_2H$. Throughout this report, the term "HFPE-1164X" denotes this specific material.

TABLE 3. CANDIDATE CARRIERS.

Halocarbon No.	HFC-227ea	HFC-236fa	HFC-236ea
Chemical Name	1,1,1,2,3,3,3-heptafluoropropane	1,1,1,3,3,3-hexafluoropropane	1,1,1,2,3,3-hexafluoropropane
Formula	CF_3CHFCF_3	$CF_3CH_2CF_3$	$CF_3CHFCHF_2$
Common/Trade Names	FM-200	FE-36	none
CAS Number	431-89-0	690-39-1	431-63-0
CCOD ID	314	442	302
Molecular Weight	170.03	152.04	152.04
Atmospheric Lifetime, years	[a]36.5	[a]209	[b]6.2
100-year GWP (CO_2 basis)	[a]2900	[a]6300	[c]n/a
LC_{50} or ALC, %	[d]>80	[d,e]>18.9	[c]n/a
NOAEL, %	[d]9	[d]10	[c]n/a
LOAEL, %	[d]10.5	[d]15	[c]n/a
Boiling Point, °C	[d,f]-16.4	[d,f]-1.4	[b]6.12
Liquid Density, 25 °C, g/mL	[g]1.395	[g]1.356	[h]1.391
Vapor Pressure, 25 °C, bar	[d]4.577	[d]2.724	[h]2.096
[i]Extinguishment Conc., vol.%	[j]6.3	[j]5.6	[j]6.6
WEq Relative to Halon 1211	2.0	1.6	1.9
SVEq Relative to Halon 1211	2.6	2.2	2.5

[a] Reference 9.
[b] Reference 10.
[c] Not available.
[d] Reference 11.
[e] ALC.
[f] At a pressure of 1 atmosphere.
[g] Reference 12.
[h] Reference 13.
[i] NMERI Standard Cup Burner, *n*-heptane fuel.
[j] Reference 14.

TABLE 3. CANDIDATE CARRIERS (CONTINUED).

Halocarbon Number	HFC-125	HFC-134a	HFC-245fa
Chemical Name	pentafluoroethane	1,1,1,2-tetrafluoroethane	1,1,1,3,3-pentafluoropropane
Formula	CHF_2CF_3	CH_2FCF_3	$CF_3CH_2CF_2H$
Common/Trade Names	FE-25	R-134a	none
CAS Number	354-33-6	811-97-2	460-73-1
CCOD ID	167	547	329
Molecular Weight	120.02	102.03	134.05
Atmospheric Lifetime, years	[a]32.6	[a]14.6	[a]6.6
100-year GWP[b] (CO_2 basis)	[a]2800	[a]1300	[b]n/a
LC_{50} or ALC, %	[c]>70	[d]56.7	[e]20
NOAEL, %	[c]7.5	[f]4	[e]20
LOAEL, %	[c]10	[f]8	[b]n/a
Boiling Point, °C	[c,g]-48.5	[h]-26.07	[i]15.2
Liquid Density, 25 °C, g/mL	[j]1.19	[j]1.209	[i]1.323
Vapor Pressure, 25 °C, bar	[c]13.71	[j]6.7	[i]1.47
[k]Extinguishment Conc., vol.%	[l]9.4	[l]10.5	[m]8.0
WEq Relative to Halon 1211	2.1	2.0	2.0
SVEq Relative to Halon 1211	3.3	3.0	2.8

[a] Reference 9.
[b] Not available.
[c] Reference 11.
[d] Reference 15.
[e] Bogdan, M., "Blowing Agents: Producer and User Perspective," International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, 17-22 December 1996.
[f] Reference 16.
[g] At a pressure of 1 atmosphere.
[h] Reference 17.
[i] Reference 18.
[j] Reference 12.
[k] NMERI Standard Cup Burner, *n*-heptane fuel.
[l] Reference 14.
[m] Work performed under this project.

TABLE 3. CANDIDATE CARRIERS (CONCLUDED).

Halocarbon No.	None	HFE-E449s1
Chemical Name	[a]hydrofluoropolyether (HFPE-1164X)	1-methoxynonafluorobutane
Formula	$HF_2CO(CF_2O)_n(CF_2CF_2O)_m CF_2H$	$CF_3CF_2CF_2 CF_2OCH_3$
Common/Trade Names	H-Galden 1164x	HFE A
CAS Number	161075-02-1	163702-07-6
CCOD ID	565	913
Molecular Weight	325	250.06
Atmospheric Lifetime, years	[b]<8	[c]4.1
100-year GWP[d] (CO_2 basis)	[b]1000 to 2000	[c]480
LC_{50} or ALC, %	[d]>3.2	[e]n/a
NOAEL, %	[d]1.2	[e]n/a
LOAEL, %	[d]1.7	[e]n/a
Boiling Point, °C	[d]100	[f]60
Liquid Density, 25 °C, g/mL	[g]1.65	[f]1.5
Vapor Pressure, 25 °C, bar	[e]n/a	[e]n/a
[h]Extinguishment Conc., vol.%	[d]5.1	~6.0
WEq Relative to Halon 1211	3.1	2.8
SVEq Relative to Halon 1211	3.5	3.5

[a] The hydrofluoropolyether (HFPE) H-Galden 1164X was supplied as an experimental sample by Ausimont S.p.A., Bollate (Milano), Italy and has an average molecular weight of 325 and a formula $HF_2CO(CF_2O)_n(CF_2CF_2O)_mCF_2H$. Throughout this report, the term "HFPE-1164X" denotes this specific material.

[b] Personal communication, to Ted A. Moore, New Mexico Engineering Research Institute, from Dr. Mario Visca, Ausimont S.p.A., Bollate (Milano), Italy, 24 October 1997.

[c] Reference 19.

[d] Reference 20.

[e] Not available.

[f] At 23 ° C. Grenfell, M. W., Klink, F. W., Owens, J. G., and Yanome, H., "New Fluorinated Solvent Alternatives," Precision Cleaning '95, Rosemont, Illinois, USA, 15-17 May 1995.

[g] Material Safety Data Sheet, Ausimont S.p.A., Bollate (Milano), Italy, 15 September 1995.

[h] NMERI Standard Cup Burner, *n*-heptane fuel.

[i] Relative to Halon 1211.

SECTION IV
TEST RESULTS

Summaries of results from the medium-scale field testing are presented in this section. Data for individual test runs are presented in Appendix B. Initially, baseline tests were performed with Halon 1211 followed by tests of neat HFPE-1164X and HFC-236fa carriers. Blends of these carriers with 1-bromopropane ($CH_3CH_2CH_2Br$, HBC-280faB1, CAS Number 106-94-5, CCOD ID 3) and with 1-bromobutane ($CH_3CH_2CH_2CH_2Br$, HBC-3-10-0oB1, CAS Number 109-65-9, CCOD ID 709, for HFC-236fa, only) were then tested.

A. HALON 1211 BASELINE DATA

Halon 1211 was tested as a baseline agent at constant flow rates, which were different for each test (Figure 3). Each data point represents an independent test. With higher flow rates, extinguishment is achieved quicker, as expected. At lower flow rates, the fire is more difficult to extinguish since less agent is being delivered per second. The minimum flow rate that is just capable of extinguishing the fire is termed the "critical flow rate." Below this critical flow rate, extinguishment cannot be achieved in a reasonable period of time (i.e., less than 20 seconds).

Figure 4 shows a plot of extinguishment time versus quantity required for extinguishment for the baseline tests. Here, linear regression has been performed to develop a curve-fit equation. Dividing the equation by time results in a curve fit to the flow rate versus extinguishment time data, as shown for Halon 1211 in Figure 3.

Developing complete data curves requires a significant amount of the test compound, and is unnecessary since only a comparison of effectiveness with other compounds is required. Since flow rate versus extinguishment time curves have similar shapes for all compounds, with extinguishment times increasing as flow rates decrease, compounds can be tested at specific flow rates and compared with Halon 1211 at those flow rates. Selection of a specific flow rate allows several tests to be performed with limited amounts of an agent.

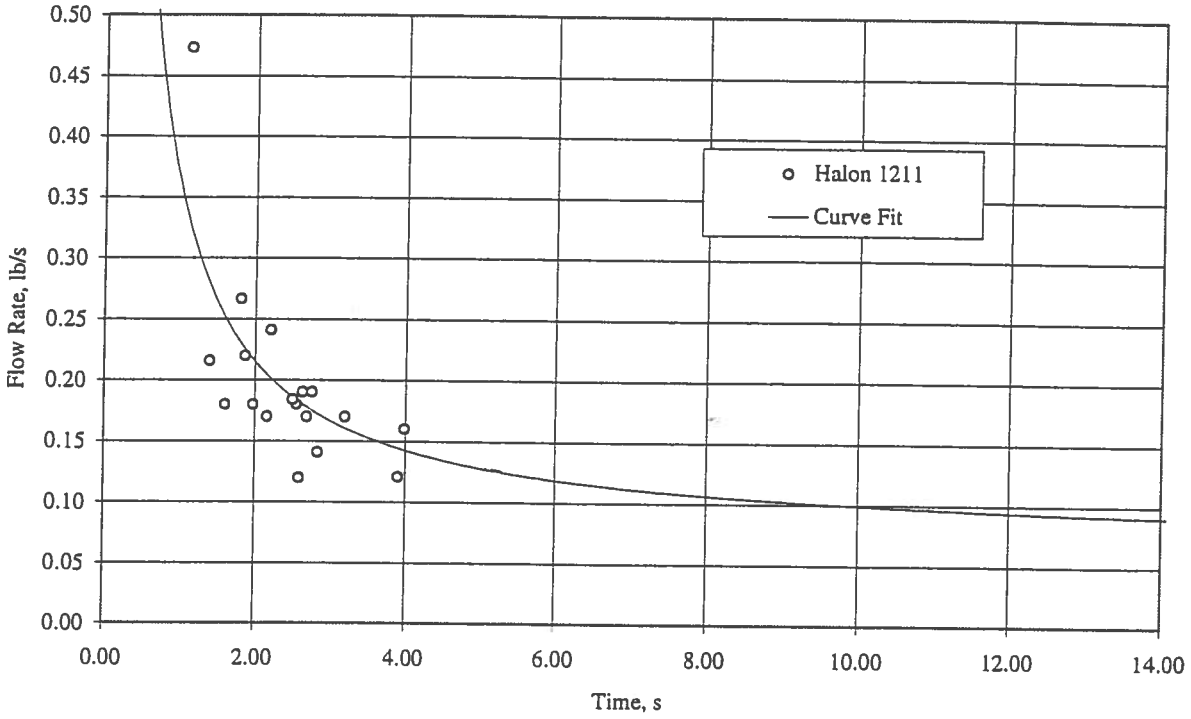

Figure 3. Flow Rate versus Extinguishment Time for Halon 1211.

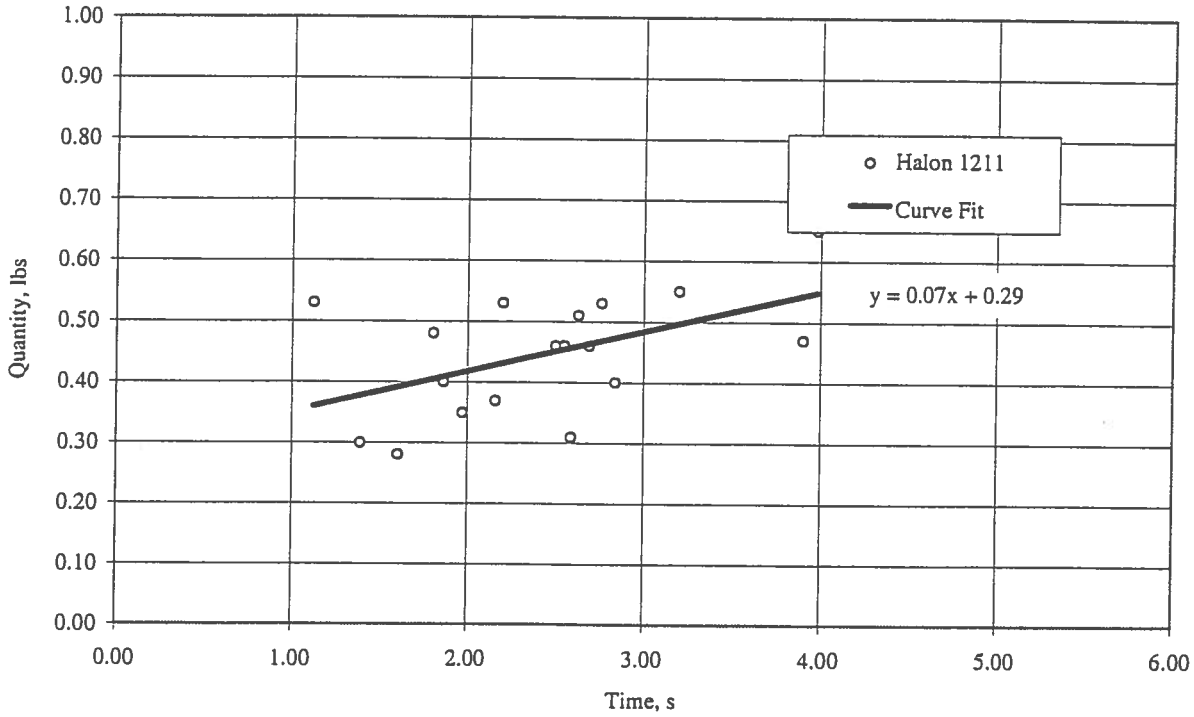

Figure 4. Quantity versus Extinguishment Time for Halon 1211.

B. HFPE-1164X/BROMOPROPANE BLENDS

The neat carrier HFPE-1164X was tested using 2.25-ft^2 (0.209-m^2) fires with the NMERI 1-Gallon (3.79-liter) Constant-Flow Extinguisher. In these tests, HFPE-1164X did not perform as well as expected based on laboratory results (Reference 1). Definitive conclusions as to why performance was poor cannot be made, however, since no efforts were made to optimize spray patterns. The spray patterns in most of the tests were relatively tight, resulting in a narrow stream and making fire extinguishment difficult.

For comparison with the neat HFPE-1164X, eight tests were performed with C_6F_{14} (perfluorohexane, FC-5-1-14, CAS Number 355-42-0, CCOD ID 178), a chemical with a high boiling point which exhibited similar performance to the HFPE-1164X in laboratory streaming experiments (Reference 1). The HFPE-1164X did not appear to be as effective as C_6F_{14}. Although HFPE-1164X did extinguish the heptane fire, the minimum flow rate capable of extinguishment was 0.38 lb/s (0.17 kg/s), as compared to 0.28 lb/s (0.13 kg/s) for perfluorohexane.

Significant enhancement over neat HFPE-1164X was achieved by blending it with 1-bromopropane. The blends appeared to be much more effective on the 2.25-ft^2 (0.209 m^2) fires than observed in laboratory-scale tests (Reference 1). As discussed in the previous paragraph, the lowest flow rate that resulted in extinguishment with pure HFPE-1164X was 0.38 lb/s (0.1 kg/s). With the addition of 25 wt.% 1-bromopropane, extinguishment was achieved at a flow rate as low as 0.29 lb/s (0.13 kg/s). Three tests were conducted with this blend, with 0.29 lb/s (0.13 kg/s) being the lowest flow rate tested. It is, therefore, quite possible that even lower flow rates could result in extinguishment.

A 10 wt.% 1-bromopropane blend with HFPE-1164X provided extinguishment at an even lower flow rate (better performance) of 0.17 lb/s (0.077 kg/s), a somewhat surprising result in light of the lower 1-bromopropane percentage. A review of the video shows that the firefighter was initially too far from the fire, and probably could have extinguished the fire as much as 3 to 4 seconds quicker. For comparison, a test was run with pure 1-bromopropane at a flow rate of 0.23 lb/s (0.10 kg/s). As observed in laboratory testing (Reference 1), pure 1-bromopropane

was discharged onto the fire for 7.5 seconds. Extinguishment was not obtained, and a large amount of smoke was produced. The amount of smoke observed in this test was significantly greater than that observed in tests with the HFPE-1164X/1-bromopropane blends.

Figure 5 compares results from medium-scale field testing for HFPE-1164X / 1-bromopropane blends with results for the neat carrier and other compounds. Numerical data for these tests are presented in Table 4.

The following can be concluded from this testing:

1. Pure HFPE-1164X does not appear to be as effective as C_6F_{14} in extinguishing fires, although extinguishment can be achieved.

2. When neat, neither 1-Bromopropane nor HFPE-1164X are highly effective in extinguishing fires; however, when blended with each other, extinguishment performance improves markedly.

3. Pure 1-bromopropane produces large volumes of smoke when applied to a fire. Blends containing 25 wt.% or less 1-bromopropane produce significantly less smoke during extinguishment.

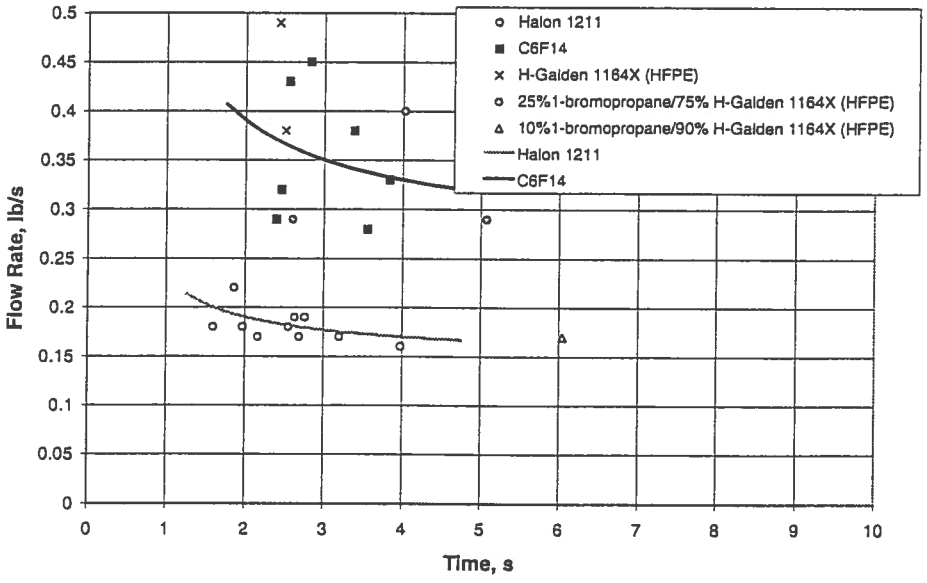

Figure 5. Flow Rate versus. Extinguishment Time for HFPE-1164X Blends and Comparison Materials.

TABLE 4. HFPE-1164X BLENDS WITH COMPARISON COMPOUNDS, 2.25-FT^2 HEPTANE FIRES.

Agent	Extinguishment quantities, lb	Extinguishment times, s	Flow rates, lb/s	Number of tests
Halon 1211	0.28 to 0.65	1.1 to 4.0	0.12 to 0.47	18
Perfluorohexane	0.7 to 1.3	2.4 to 3.8	0.28 to 0.45	7
HFPE-1164X	0.94, 1.22	2.4, 2.5	0.38, 0.49	2
1-Bromopropane	N/A	N/A	0.23	1
25% 1-Bromopropane 75% HFPE-1164X	0.76 to 1.61	2.6 to 5.1	0.29 to 0.40	3
10% 1-Bromopropane 90% HFPE-1164X	1.02	6.04	0.17	1

C. HFC-236FA/BROMOALKANE BLENDS

Tests using 2.25-ft^2 (0.209-m^2) fires with heptane fuel were performed with pure HFC-236fa and blends of HFC-236fa with 1-bromopropane and 1-bromobutane. The NMERI 1-Gallon (3.79-liter) Constant-Flow Rate Extinguisher test apparatus was used with halon nozzles, providing relatively effective spray patterns.

Tests with HFC-236fa and 1-bromopropane blends were performed with 1-bromopropane concentrations of 10, 15, and 25 wt.%. Figure 6 and Figure 7 show plots of the test data and curve fits. A discussion on how the curve fits are developed is presented in Section A, Halon 1211 Baseline Tests. Table 5 summarizes the data.

A significant enhancement is seen with the addition of 1-bromopropane to HFC-236fa. With 10 wt.%, 15 wt.%, and 25 wt.% 1-bromopropane, extinguishment quantities ranged from 0.7 to 1.1 pounds (0.3 to 0.50 kilograms), compared to 1.7 to 2.6 pounds (0.77 to 1.2 kilograms) for the pure HFC-236fa. The flow rates ranged from 0.15 to 0.22 lb/s (0.068 to 0.10 kg/s) for both the pure chemical and the blends. Overall, addition of 1-bromopropane reduced the average quantities of agent required for extinguishment by more than 50 percent (e.g., HFC-236fa compared with HFC-136fa/1-bromopropane. A similar enhancement was seen with a 15 wt.% blend of 1-bromobutane in HFC-236fa.

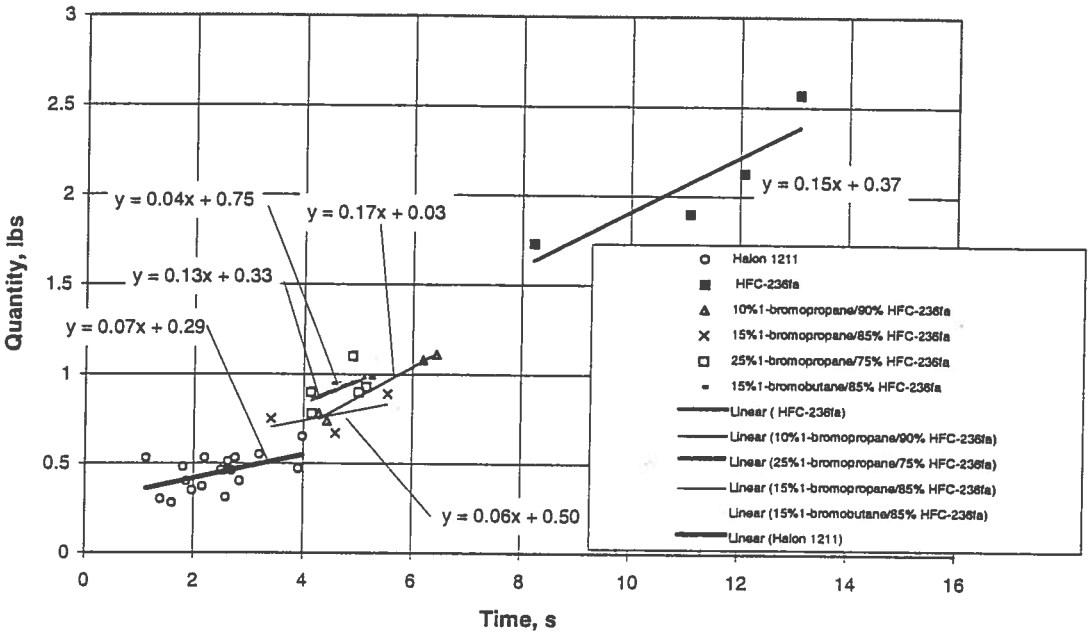

Figure 6. Quantity versus Extinguishment Time for HFC-236fa Blends and Comparison Materials.

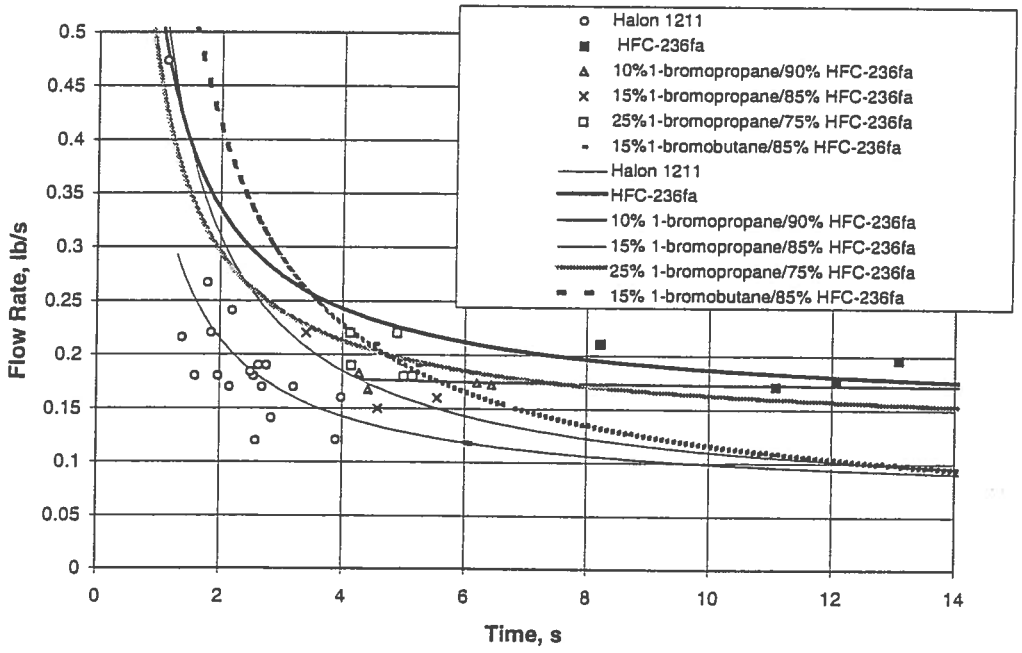

Figure 7. Flow Rate versus Extinguishment Time for HFC-236fa Blends and Comparison Materials.

TABLE 5. SUMMARY OF HFC-236fa AND HFC-236fa/BROMOALKANE TESTS.

Agent	Extinguishment quantities, lb	Extinguishment times, s	Flow rates, lb/s	Number of tests
Halon 1211	0.28 to 0.65	1.1 to 4.0	0.12 to 0.47	18
HFC-236fa	1.73 to 2.57	8.2 to 13.1	0.17 to 0.21	4
10% 1-Bromopropane 90% HFC-236fa	0.74 to 1.11	4.3 to 6.4	0.17 to 0.18	4
15% 1-Bromopropane 85% HFC-236fa	0.67 to 0.89	3.4 to 5.5	0.15 to 0.22	3
25% 1-Bromopropane 75% HFC-236fa	0.78 to 1.10	4.1 to 5.1	0.18 to 0.22	5
15% 1-Bromobutane 85% HFC-236fa	0.95, 0.98	4.5, 5.2	0.19, 0.21	2

D. ADDITIONAL BROMOALKANE BLEND TESTING

The test results above were similar to those obtained in testing for the U.S. Army, which is currently seeking a replacement for CO_2 in their portable extinguishers. NMERI performed an extensive test series on 5-ft^2 (0.46-m^2) Jet-A fires (Underwriters Laboratories (UL) 2B) under a separate contract to determine the effectiveness of agents that included HFC-236fa, HFC-227ea, HFPE-1164X, and each of these blended with 1-bromopropane, on larger fires. Although the test fuel was Jet-A, a similar decrease in quantity required for extinguishment compared with neat carriers was seen with the addition of the 1-bromopropane. Details of the testing are discussed in Reference 21, and the results are summarized in Table 6.*

Although little can be inferred from the 12.5-ft^2 (1.16-m^2) (Underwriters Laboratories (UL) 5B) fire tests, where only two extinguishments were obtained (Table 7, all at ambient temperature), it is interesting to note that this size fire was extinguished once with the HFPE-1164X and with none of the other neat agents. This indicates that HFPE-1164X may be a promising streaming agent for larger fires, due to its low vapor pressure. The only other agent with which extinguishment was attained was a blend of HFC-236fa and 1-bromopropane.

* The U.S. Army Tank-Automotive and Armament Command (TACOM) has granted permission to include these data.

TABLE 6. SUMMARY OF 5-FT^2 (0.46-M^2) JET-A FIRE TESTING USING ARMY EXTINGUISHERS.

Agent	Temperature, °C	Extinguishment quantity range, lb	Extinguishment quantity, average, lb	Percent fires extinguished, %
HFC-236fa	ambient	1.91 to 2.32	2.06	100 (3 of 3)
HFC-236fa	-45.6	1.76 to 2.14	1.93	100 (3 of 3)
HFC-236fa	60	1.70 to 1.96	1.83	100 (2 of 2)
HFC-227ea	ambient	1.30 to 2.40	1.63	100 (4 of 4)
HFC-227ea	-45.6	1.29 to 1.44	1.35	100 (3 of 3)
HFC-227ea	60	1.08 to 1.95	1.52	100 (2 of 2)
HFPE-1164X	ambient	2.21 to 4.60	2.97	73 (11 of 15)
HFPE-1164X	-45.6	2.1	2.10	100 (1 of 1)
HFPE-1164X	60	2.31 to 3.78	3.01	100 (3 of 3)
CO_2	ambient	0.98 to 1.69	1.32	100 (3 of 3)
10% 1-Bromopropane 90% HFPE-1164X	ambient	1.79 to 2.96	2.29	100 (4 of 4)
15% 1-Bromopropane 85% HFC-227ea	ambient	1.08	1.08	100 (1 of 1)
15% 1-Bromobutane 85% HFC-227ea	ambient	1.70	1.70	100 (1 of 1)

E. CYCLOTRIPHOSPHAZENE TESTING

A cyclotriphosphazene fluid, $[P_3N_3(OCH_2CF_3)_{3.5}(OC_6H_5)_{1.25}(m\text{-}OC_6H_4CH_3)_{0.87}\text{-}(p\text{-}OC_6H_4CH_3)_{0.37}]$, was obtained from the U.S. Navy and tested on a 2.25-ft^2 (0.209-m^2) heptane fire. Initially, a test was attempted using 1.2 pounds (0.54 kilograms) of the fluid in a nominal 1.25-pound (0.567-kilogram) halon extinguisher. The largest nozzle available, with an orifice diameter of 0.098 inch (2.5 millimeter), and a nitrogen pressure of 125 lb$_f$/in^2 (862 kPa) were used. The average flow rate obtained was 0.23 lb/s (0.104 kg/s). The spray pattern, which had a tight (not well-dispersed) stream, was not optimum. Nevertheless, the compound demonstrated no extinguishing capabilities.

TABLE 7. SUMMARY OF 12.5-FT^2 (1.16 M^2) JET-A TEST FIRES USING ARMY EXTINGUISHERS.

Agent	Extinguishment quantity, avg., lb	Percent fires extinguished, %
HFC-236fa	N/A	0 (0 of 1)
HFC-227ea	N/A	0 (0 of 3)
HFPE-1164X	2.8	25 (1 of 4)
CO_2	N/A	0 (0 of 3)
15% 1-Bromopropane 85% HFPE-1164X	N/A	0 (0 of 2)
15% 1-Bromopropane 85% HFC-227ea	N/A	0 (0 of 1)
15% 1-Bromopropane 85% HFC-236fa	3.14	100 (1 of 1)

In a following test, the NMERI 1-Gallon (3.79-liter) Constant-Flow Rate Extinguisher (Reference 22) was utilized, and the cyclotriphosphazene fluid was blended with HFPE-1164X. Several tests were performed using the 2.25-ft^2 (0.209-m^2) fire, and again, the cyclotriphosphazene fluid showed no extinguishment enhancement compared to the HFPE-1164X alone. The high viscosity of the cyclotriphosphazene made reasonable flow rates unattainable. The lack of fluorination may explain the poor performance of this cyclotriphosphazene. Other phosphazenes tested in the cup-burner in the initial stages of this project (Reference 1) were fluorinated, however, quantities large enough for medium-scale testing were not available.

SECTION V
CONCLUSIONS AND RECOMMENDATIONS

A. CONCLUSIONS

Blends of bromoalkanes (especially 1-bromopropane) with HFC-236fa and HFPE-1164X have an enhanced fire suppression capability compared to the neat carriers. This enhancement was significant on 2.25-ft^2 (0.209-m^2) heptane fires, reducing the agent required for extinguishment by 50 percent at similar flow rates. Tests performed for the U.S. Army on 5-ft^2 and 12.5-ft^2 (2.32-m^2 and 1.16-m^2) Jet-A fuel fires utilizing HFC-227ea, HFC-236fa, and HFPE-1164X blended with 1-bromopropane showed similar enhancement.

Cyclotriphosphazene fluid, $[P_3N_3(OCH_2CF_3)_{3.5}(OC_6H_5)_{1.25}(m\text{-}OC_6H_4CH_3)_{0.87}\text{-}(p\text{-}OC_6H_4CH_3)_{0.37}]$ did not appear to be effective at extinguishing the fire. This particular cyclotriphosphazene, which was obtained from the U.S. Navy, was very viscous and the spray pattern was tight and not well-dispersed. Nevertheless, the compound did not appear to demonstrate any extinguishing capabilities. The lack of fluorination may explain the poor performance of this cyclotriphosphazene. Other phosphazenes tested in the cup-burner in the initial stages of this project were fluorinated, however, quantities large enough for medium scale testing were not available.

B. RECOMMENDATIONS

Tests should be performed with 1-bromopropane blended with HFC-236fa and HFPE-1164X on larger-scale heptane and Jet-A fires, including 12.5-ft^2 (1.16 m^2) (UL-5B) and 25-ft^2 (2.32-m^2) (UL-10B) fires. With these fire sizes, existing UL-approved halon-type extinguishers should be used, and comparisons made with currently available halon replacement UL-approved extinguishers. It is important that proper nozzles, fill densities, and nitrogen pressures are used to obtain optimum performance. Appendix C provides recommendations and suggestions for nozzle design and filling considerations when conducting larger size fires using portable extinguishers. Constant flow extinguishers with larger nozzles could also be utilized.

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APPENDIX A
HALOCARBON NOMENCLATURE

IUPAC NOMENCLATURE

The International Union of Pure and Applied Chemistry (IUPAC) has developed rules for naming organic compounds. It is assumed that the reader is familiar with the basics of these rules. The following is only a brief overview of some of the points about the IUPAC system of particular importance to naming halocarbons.

In the IUPAC naming system, each substituent is assigned a number giving its position on the molecule, unless no ambiguity is caused omitting the number. For example, fluoroethane, CH_3CH_2F, requires no numbering since the same compound results no matter where the fluorine atom is place. On the other hand, 1-fluoropropane, $CH_2FCH_2CH_3$, requires a number to distinguish it from 2-fluoropropane, CH_3CHFCH_3. If more than one of a given substituent is present, the prefixes di-, tri-, tetra-, penta-, and so forth are used.

The carbon chain of the molecule is numbered to give the lowest sum of numbers to the substituents. For example, the molecule $CH_2ClCHClCHCl_2$ is named 1,1,2,3-tetrachloropropane (numbered from the right), not 1,2,3,3-tetrachloropropane. If the numbering (and therefore the sum of substituent numbers) would be the same from either end, the first group alphabetically takes priority. Thus, CH_2FCH_2I is named 1-fluoro-2-iodoethane (not 2-fluoro-1-iodoethane). Similarly, because chlorine comes before fluorine in the alphabet, $CHF_2CHClCHClF$ is designated 1,2-dichloro-1,3,3-trifluoroethane (not 2,3-dichloro-1,1,3-trifluoroethane) even though the set of numbers is the same (1,1,2,3,3) from either end of the molecule.

Prefixes such as di-, tri-, tetra-, etc. are ignored in the alphabetization of substituents. These prefixes are inserted after the substituent names, such as "bromo," "chloro," "fluoro," and "iodo," have been alphabetized. Therefore, "bromo" always comes before "chloro," no matter how many of each are present. For example the compound $CHBr_2CBrCl_2$ is named 1,2,2-tribromo-1,1-dichloroethane (not 1,1-dichloro-1,2,2-tribromoethane).

If a conflict in priority between numbering and alphabetization occurs, numbering takes precedence. The carbon atoms are numbered to give the lowest set of substituent numbers, instead of the lowest number going to the carbon with the first alphabetical substituent. For example, $CHCl_2CF_3$ is called 2,2-dichloro-1,1,1-trifluoroethane, the lowest set of numbers taking priority. It would be incorrect to name this compound 1,1-dichloro-2,2,2-trifluoroethane, giving priority in numbering carbon atoms to the substituent names.

The prefix "per" indicates that every possible site on the carbon skeleton is occupied by the same type of substituent. For example, perfluoropropane is $CF_3CF_2CF_3$.

HALOCARBON NUMBERING SYSTEM

It has become a general practice within the refrigeration industry to designate various halocarbons with a number. This "Halocarbon Numbering System" has now become widely used, and an unofficial extended version has been used in both national and international regulations. The Halocarbon Numbering System (sometimes called the CFC, Freon®, or Refrigerant Numbering System) was developed by DuPont for Freon® chemicals in the late 1930s. The system was later expanded and formalized into a standard by the American Society of Heating, Refrigerating, and Air-Conditioning Engineers (ASHRAE) and the American National Standards Institute (ANSI) (*Number Designation and Safety Classification of Refrigerants*, ANSI/ASHRAE Standard 34-1992, American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc., Atlanta, Georgia, 1992). Note, however, that this Standard uses the Halocarbon Numbering System only for derivatives of cyclobutane, propane, ethane, and methane. The unofficial, but widely used, extended numbering system described in this document is applicable for larger molecules; however, this will give numbers that could conflict with refrigerant numbers assigned to other chemicals (particularly, blends or inorganics). Neither the method described in ANSI/ASHRAE Standard 34-1992, nor the extended method described here allows the assignment of halocarbon numbers to branched compounds (i.e., compounds that contain carbon atoms located in other than a single chain or a single ring).

In the early days, many of the halocarbon chemicals used as refrigerants were given numbers preceded by the designation "Freon®"; however, since this is a trade name, other

prefixes are now usually used. In the refrigeration industry, it is common practice to precede the Halocarbon Number with an "R." However, such a prefix can be misleading for refrigerants other than butane, propane, ethane, or methane derivatives. Series of letters, termed "Composition-Designating Prefixes" in the ANSI/ASHRAE Standard 34-1992, denoting the type of compound are now often used. For example, compounds containing only chlorine and fluorine (in addition to carbon) have numbers preceded by "CFC," which stands for "chlorofluorocarbon." Though not universally accepted or standardized, other prefixes are being increasingly used. Table A-1 lists most of the prefixes that have been adopted for non-ether halocarbons. The Composition-Designating Prefix "FC" is used for perfluorocarbons; however, the generic term "PFC" is often used for the perfluorocarbon family.

In the Halocarbon Numbering System, the first number gives the number of carbon atoms minus one, followed by (in order) the number of hydrogen atoms plus one and the number of fluorine atoms:

first number	number of carbon atoms - 1
second number	number of hydrogen atoms + 1
third number	number of fluorine atoms

All remaining atoms are assumed to be chlorine atoms. An initial zero (indicating a one-carbon compound) is omitted. For example, CFC-12 has one carbon atom (the initial zero has been dropped), no hydrogen atoms (0 + 1 = 1), two fluorine atoms and, by default, two chlorine atoms, for a formula CF_2Cl_2. CFC-113 is CF_3CCl_3 or one of its isomers. When any number in the halocarbon designation contains two or more digits, dashes are used to separate the numbers. For example, $CF_3CF_2CF_2CF_2CClF_2$ is CFC-4-1-11 (ignoring isomer designations discussed below). It has been suggested that dashes be used only to set off the specific numbers with multiple digits, but this could be misleading. For example, CFC-41-11 could correspond to a 5-carbon compound or a 42-carbon compound (admittedly, unlikely).

TABLE A-1. COMPOSITION-DESIGNATING PREFIXES FOR HALOCARBON NUMBERS.

Prefix	Elements in Chemical	Chemical Family
BC	Br, C	Bromocarbon
BCC	Br, Cl, C	Bromochlorocarbon
BCIC	Br, Cl, I, C	Bromochloroiodocarbon
BCFC	Br, Cl, F, C	Bromochlorofluorocarbon
BCFIC	Br, Cl, F, Cl, C	Bromochlorofluoroiodocarbon
BFC	Br, F, C	Bromofluorocarbon
BFIC	Br, F, I, C	Bromofluoroiodocarbon
BIC	Br, I, C	Bromoiodocarbon
CC	Cl, C	Chlorocarbon
CFC	Cl, F, C	Chlorofluorocarbon
CFIC	Cl, F, I, C	Chlorofluoroiodocarbon
CIC	Cl, I, C	Chloroiodocarbon
FC	F, C	(Per)fluorocarbon
FIC	F, I, C	Fluoroiodocarbon
HBC	H, Br, C	Hydrobromocarbon
HBCC	H, Br, Cl, C	Hydrobromochlorocarbon
HBCFC	H, Br, Cl, F, C	Hydrobromochlorofluorocarbon
HBCFIC	H, Br, Cl, F, I, C	Hydrobromochlorofluoroiodocarbon
HBCIC	H, Br, Cl, I, C	Hydrobromochloroiodocarbon
HBFC	H, Br, F, C	Hydrobromofluorocarbon
HBFIC	H, Br, F, I, C	Hydrobromofluoroiodocarbon
HBIC	H, Br, I, C	Hydrobromoiodocarbon
HC	H, C	Hydrocarbon
HCC	H, Cl, C	Hydrochlorocarbon
HCFC	H, Cl, F, C	Hydrochlorofluorocarbon
HCFIC	H, Cl, F, I, C	Hydrochlorofluoroiodocarbon
HCIC	H, Cl, I, C	Hydrochloroiodocarbon
HFC	H, F, C	Hydrofluorocarbon
HFIC	H, F, I, C	Hydrofluoroiodocarbon
HIC	H, I, C	Hydroiodocarbon
IC	I, C	Iodocarbon

For cyclic compounds, the prefix "C" precedes the Halocarbon Number. For example, perfluorocyclobutane (cyclo-C_4F_8) is FC-C318. For unsaturated compounds, a number giving the number of double bonds is added on the left. Thus CF_2=CClF is CFC-1113. The presence of four numbers (may be more than four digits) always denotes an unsaturated compound.

Two-Carbon Compounds (Ethane and Ethene Derivatives)

When there are two (or more) carbon atoms present, isomers are possible, and these may have identical Halocarbon Numbers. To distinguish these isomers for ethane derivatives, a lower case letter is added based on the difference in the sum of the atomic masses of the carbon substituents. The designation for the isomer with the smallest difference in the sum of the masses on the two carbon atoms has no letter; the designation corresponding to the next smallest difference has an "a", the next a "b", etc. Some examples are given below for the isomers of dichlorodifluoroethane.

$CHClFCHClF$	HCFC-132
$CHCl_2CHF_2$	HCFC-132a
$CClF_2CH_2Cl$	HCFC-132b
CCl_2FCH_2F	HCFC-132c

If bromine is present in the molecule, the Halocarbon Number is first assigned as if the bromine atoms were chlorine atoms (i.e., the Halocarbon Number is assigned for the "parent" molecule). The designation "Bn," where "n" is the number of bromine atoms, is then added to the end of the Halocarbon Number. For example, the anesthetic Halothane ($CF_3CHBrCl$) is HBCFC-123B1. The absence of a small letter indicates that this is the most symmetrical isomer, and the final "B1" means that one of the chlorine atoms was replaced with a bromine. The parent compound in this case is CF_3CHCl_2 (HCFC-123). As another example, $CClF_2CHBrF$, parent compound $CClF_2CHClF$, is HBCFC-123aB1 (omitting a final suffix for the bromine position, which is discussed below). CGET/NMERI has extended this further to include iodine compounds using a suffix "In," where "n" is the number of iodine atoms. This extension gives FIC-12I2 for CF_2I_2 and BFIC-12B1I1 for CF_2BrI.

Where the positions of the bromine atoms are ambiguous, Greek letter suffixes are added. The letters "α," and "β" denote the carbon atoms in the chain starting from the end

carbon having the highest sum of atomic weights in the parent compound. HBCFC-123aB1 exists as two isomers — HBCFC-123aB1α ($CBrF_2CHClF$) and HBCFC-123aB1β ($CClF_2CHBrF$). Similarly, $CBrClFCBrF_2$ is HBCFC-113B2αβ and CBr_2FCClF_2 is HBCFC-113B2αα. NMERI/CGET has extended this to iodine-containing compounds: $CF_2ICHClF$ is HCFIC-123aI1α, $CClF_2CHFI$ is HCFIC-123aI1β, $CClFICF_2I$ is CFIC-113I2αβ, and CFI_2CClF_2 is CFIC-113I2αα. Where both bromine and iodine are present, the Greek letter position designations are placed after the appropriate designations giving the number of bromine and iodine atoms. For example, $CClFICBrF_2$ is BCFIC-113B1βI1α and $CBrClFCIF_2$ is BCFIC-113B1αI1β.

Three-Carbon Compounds (Propane, Cyclopropane, and Propene Derivatives)

The Halocarbon Numbering System for linear three-carbon compounds (propanes) is similar to that for two-carbon compounds; however, two letters are required to specify the isomer. (Letters are omitted when there is no possibility of isomerism.) The first letter refers to the central (methylene) carbon atom of the propane. To assign this letter, one calculates the combined atomic mass of the substituents on this carbon atom in the parent compound (containing only H, F, and/or Cl). The letter "a" represents the largest mass possible, the letter "b," the next largest, etc. The letters are assigned as shown in Table A-2.

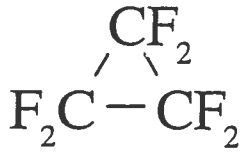
The second letter is determined by the difference in the combined atomic masses of the substituents on the two terminal carbon atoms. The smallest difference is assigned the letter "a," the next smallest difference is assigned the letter "b," followed by "c," "d," etc. This method of isomer designation differs from that for two-carbon compounds, in which the smallest difference has no letter. For example, $CHCl_2CF_2CF_3$ (3,3-dichloro-1,1,1,2,2-pentafluoro-propane) is designated HCFC-225ca, and the isomer $CHClFCF_2CClF_2$ (1,3-dichloro-1,1,2,2,3-pentafluoropropane) is HCFC-225cb. Where the number alone uniquely defines the structure, suffix letters are not used. Thus, $CF_3CF_2CF_3$ is FC-218, not FC-218ca.

TABLE A-2. METHYLENE CARBON DESIGNATIONS.

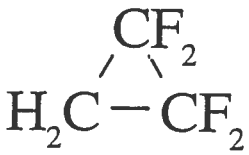
Suffix	Chemical Group
a	$-CCl_2-$
b	-CClF-
c	$-CF_2-$
d	-CHCl-
e	-CHF-
f	$-CH_2-$

If a linear three-carbon compound contains bromine or iodine, the suffix "Bn" or "In," where "n" is the number of bromine or iodine atoms, is added as done for methane and ethane derivatives. Where the positions of the bromine or iodine atom are ambiguous, Greek letter suffixes are again added. The letters "α," "β," and "γ" denote the carbon atoms in the chain starting from the end carbon having the highest sum of atomic weights in the parent compound. Thus, $CF_3CBrClCH_2Br$ (parent compound, $CF_3CCl_2CH_2Cl$) is HBCFC-233abB2βγ and $CF_3CHClCHI_2$ (parent compound $CF_3CHClCHCl_2$) is HBCFC-233daI2ααα. Application to mixed bromine/iodine derivatives is obvious: $CF_3CFBrCF_2I$ is BFIC-216baB1βI1α, $CF_3CFICBrF_2$ is BFIC-216baB1αI1β, and $CF_3CBrICF_3$ is BFIC-216aaB1I1. Note that the last compound is not designated as BFIC-216aaB1βI1β since the iodine and bromine must reside on the central atom for a compound with the Halocarbon Number 216aa. Isomer designations for the bromine or iodine positions are always omitted when no ambiguity can result.

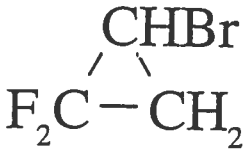
For halogenated derivatives of cyclopropane, the carbon atom containing the largest sum of atomic masses for attached substituents in the parent compound is designated as the "central" carbon atom (carbon atom 2). The designation system as described above for linear propanes is then used, treating the cyclic compound as a linear compound. Six examples are shown below.



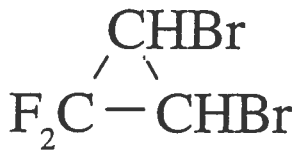
FC-C216



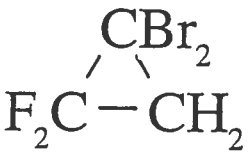
HFC-C234cb



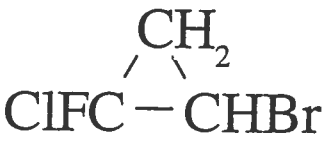
HBFC-C242caB1



HBFC-C232caB2



HBFC-C232abB2



HBCFC-C241baB1α

Halocarbon designations for propenes contain four numbers starting with 1 (one double bond) and two lower case letter suffixes. The first suffix designates the single atom attached to the central atom (methine group, Table A-3). The second letter gives the substitution on the terminal methylene carbon atom using the same letter designations as used for the central methylene carbon on propane derivatives (Table A-2). Thus, $CH_2=CHCF_2Cl$ is HCFC-1242zf. Bromo- and iodopropenes are designated in the same way as for bromo- and iodopropanes and bromo- and iodoethanes (i.e., with suffixes "Bn" and "In." Greek letters are added where necessary starting with the methylene end. Thus $CH_2=CBrCF_2Br$ (parent compound, $CH_2=CClCF_2Cl$) is HBFC-1232xfB2 (no Greek Letter descriptor is needed since the positions of the bromine atoms are fixed by the Halocarbon Number) and $CHI=CBrCClF_2$ (parent compound, $CHCl=CClCF_2Cl$)l is HBCFIC-1222xdB1βI1α. At this time, no procedures have been established for designating Halocarbon Numbers for unsaturated cyclic compounds.

Compounds with Four or More Carbon Atoms

Root numbers are assigned to linear compounds with four or more carbon atoms in a way similar to that used for compounds with fewer carbon atoms. To differentiate between isomers, carbon atoms containing a single substituent (methine carbons) are designated as shown in Table A-3, carbon atoms with two substituents (methylene carbons) as shown in Table A-2, and methyl groups as in Table A-3. Methine Carbon Designations.

Suffix	Chemical Group
x	–CCl
y	–CF
z	–CH

Some examples for larger molecules are shown in Table A-5. Note again that isomer designation letters not needed to describe a structure are omitted. Thus, CCl3CCl2CCl2CCl2CCl3 is designated as CC-410 and not as CC-410jaaaj. Similarly, CCl3CF2CF2CF2CF3 is CFC-419j; no additional letters are needed to describe the structure.

Cyclic compounds containing four or more atoms require an arbitrary rule to select an end carbon atom. Here, we propose that the atom that allows the lowest alphabetical sequence be designated as the number 1 atom. This same carbon should then be used as the number 1 carbon for determining the location of bromine atoms, where necessary. Some examples are shown below. Note that, as usual, letters are omitted when no ambiguity can result.

Table A-4. Letter designations begin at one end of the molecule, which is chosen to keep the alphabetical sequence (first, the number of letters and, then, the letters themselves) as low as possible. Bromine- and/or iodine-substituted compounds are handled in a fashion similar to that used for compounds with three or fewer carbon atoms.

TABLE A-3. METHINE CARBON DESIGNATIONS.

Suffix	Chemical Group
x	
y	
z	

Some examples for larger molecules are shown in Table A-5. Note again that isomer designation letters not needed to describe a structure are omitted. Thus, $CCl_3CCl_2CCl_2CCl_2CCl_3$ is designated as CC-410 and not as CC-410jaaaj. Similarly, $CCl_3CF_2CF_2CF_2CF_3$ is CFC-419j; no additional letters are needed to describe the structure.

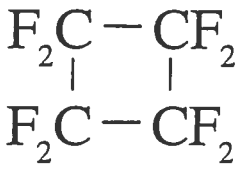
Cyclic compounds containing four or more atoms require an arbitrary rule to select an end carbon atom. Here, we propose that the atom that allows the lowest alphabetical sequence be designated as the number 1 atom. This same carbon should then be used as the number 1 carbon for determining the location of bromine atoms, where necessary. Some examples are shown below. Note that, as usual, letters are omitted when no ambiguity can result.

TABLE A-4. METHYL GROUP DESIGNATIONS.

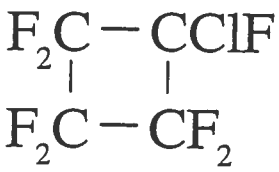
Suffix	Chemical Group
j	$-CCl_3$
k	$-CCl_2F$
l	$-CClF_2$
m	$-CF_3$
n	$-CHCl_2$
o	$-CH_2Cl$
p	$-CHF_2$
q	$-CH_2F$
r	-CHClF
s	$-CH_3$
t	–C

TABLE A-5. EXAMPLES FOR COMPOUNDS WITH FOUR OR MORE CARBON ATOMS.

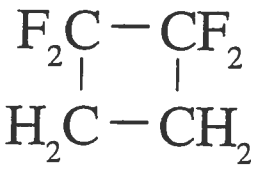
Compound	Halocarbon Number
$CCl_3CCl_2CCl_2CCl_2CCl_3$	CC-410
$CCl_3CF_2CF_2CF_2CF_3$	CFC-419j
$CF_3CClFCH_2CH_2F$	HCFC-355mb
$CF_3CBrFCH_2CH_2F$	HBFC-355mbfB1
$CF_3CHFCHFCF_2CF_3$	HFC-4-3-10mee
$CF_3CF_2CH_2CH_2F$	HFC-356mcf
$CF_2=CFCH=CH_2$	HFC-2343cy



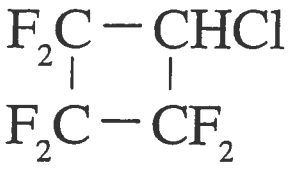
FC-C318



CFC-C317



HFC-C354cc



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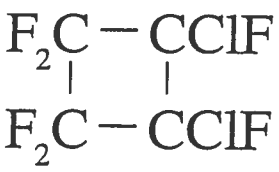
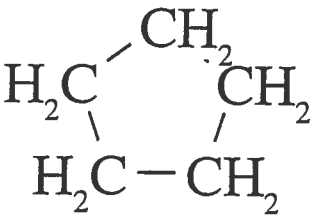
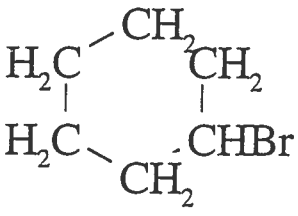


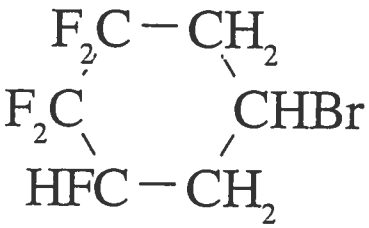
CFC-C316bb



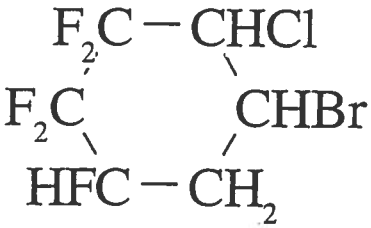
HC-C4-11-0



HBC-C5-12-0B1



HBFC-C575efdfB1



HBCFC-C565ddfeB1β

Ethers

Ether designations have an "E" or "CE" (in the case of cyclic ethers) immediately preceding designation number. The Composition-Designating Prefixes are the same as those for the corresponding halocarbons in Table A-1 except that an the letter "C" for carbon is replaced

by the letter "E" for ether. For dimethylether derivatives, designations are derived in the same way as those for the haloethanes and no further suffixes are needed.

For straight-chain, three-carbon derivatives, the root number and suffix letters are determined as for the propanes and propenes. The position(s) of the oxygen atom(s) is designated as follows. The carbon atoms are numbered sequentially with "1" assigned to the end carbon with the largest number of hydrogen atoms. When the end carbon atoms contain the same number of hydrogen atoms, number 1 is assigned to the end carbon having the largest number of iodine, then bromine, then chlorine, and finally fluorine atoms. (If the molecule is symmetrical, there is no need to distinguish between the two end carbon atoms, and the ether position number is assigned as 1.) The number giving the location of the ether oxygen is placed at the end of the suffix letters, which are retained when a single isomer exists. Some examples follow: CF_3-O-CF_2CF_3, FE-E218ca1; CHF_2-O-$CHClCHF_2$, HCFE-E244da1; CF_3-O-CH_2CHF_2, HFE-E245fa2; CF_3-O-CH_2-O-CHF_2, HFE-E245fa12; CF_3-O-$CF=CF_2$, FE-E1216yc1; and CHF_2-O-$CCl=CF_2$, HCFE-E1244xc1. This can be extended to bromine- (and iodine-) containing three-carbon ethers by placing "Bn," where "n" is the number of bromine atoms, following the number designating the ether oxygen location as shown in the following examples: CF_3-O-CF_2CBrF_2, FE-217ca2B1; CF_3-O-$CBrFCF_3$, FE-217ba1B1; and CF_3-O-CBr=CHF, FE-1224xe1B1. When the specific location of a bromine (and/or iodine) must be designated, the numbering system described earlier for Greek letter suffixes is used (i.e., the end carbon having the highest sum of atomic weights in the parent compound assigned as 1). Note that this differs from the numbering system used for the assignment of the position of the ether oxygen. The following are examples for bromine-containing ethers, where the specific bromine position must be designated: CHClF-O-$CBrFCF_3$, HBCFE-E225ba1B1β; CHBrF-O-$CClFCF_3$, HBCFE-E225ba1B1γ; and CHBrF-O-$CCl=CF_2$, HBCFE-E1223xc1B1γ. Nomenclature rules have been established in the ANSI/ASHRAE Standard 34-1992 for only 3-carbon cyclic ethers containing a single oxygen atom. For such compounds, the oxygen atom is taken to be positioned between C1 and C3 and the remaining chain is designated using the procedure employed for propanes. The location of the ether oxygen is not given. Thus, -CF_2CHFCF_2-O- is HFE-CE225ea, -$CF_2CBrFCFBr$-O- is HBFE-CE214baB2, and -$CF_2CClFCFBr$-O- is HBCFE-CE214baB1α. At this time, no rules have been established or are proposed here for cyclic ethers containing multiple oxygen atoms.

We can modify the established rules to include linear and cyclic ether molecules containing four or more carbon atoms by using methods analogous to those shown above. Thus, the ether oxygen atoms are temporarily eliminated, and the remaining chain is assigned a designation number and isomer suffixes as described earlier. The position of the oxygen atom in cyclic ethers is fixed and need not be given. Some examples for cyclic ethers follow: cyclo -O-$CF_2CF_2CF_2CF_2$-. FE-CE318; cyclo -O-$CF_2CBrFCF_2CF_2$-, BFE-CE317cbB1; cyclo --O-$CH_2CF_2CBrFCH_2$-, HBFE-CE353sbcB1. When determining the location for the ether oxygen and when there is no distinction between the end carbon atoms based on the number of hydrogen atoms (followed by number of iodine, bromine, chlorine, and fluorine atoms), proceed to the next carbon atom until a difference between the two ends appears. Thus, CHF_2-O-$CH_2CF_2CHF_2$ is HFE-E356pfc1 and not HFE-E356pfc2. Again the ether positions in linear compounds are located starting with the carbon containing the largest number of hydrogen atoms (followed, as needed, by the largest numbers of iodine, bromine, chlorine, and fluorine atoms). Examples are given in Table A-6. As is the case for cyclopropanes, the present methods do not allow designations for cyclic ethers containing multiple oxygen atoms.

TABLE A-6. EXAMPLES FOR ETHERS WITH FOUR OR MORE CARBON ATOMS.

Compound	Halocarbon Number
$CF_3CF_2CF_2CF_2$-O-CH_3	HFE-E449s1
$CF_3CF_2CF_2CF_2$-O-CH_2CH_3	HFE-E569sf2
CF_3CH_2-O-CH_2CF_2Br	HBFE-E355lff2B1
CF_3CHCl-O-CH_2CF_2Br	HBFE-E355lfd2B1β
$CF_3CF=CFCF_2$-O-CH_3	HFE-E1447scy1
CF_3CH_2-O-$CH=CH_2$	HFE-E1363mc2
CHF_2CF_2-O-$CH_2CH=CH_2$	HFE-E1474pcf3
CHF_2CF_2-O-$CH=CH_2$	HFE-E1354pc2
CF_3-O-$CH=CCl$-O-CF_3	HCFE-E1326mxz13
$CH_2BrCH=CFCF_2$-O-CH_3	HFBE-E1473ozyc1B1
CF3-O-CBrClCHBr-O-CF3	HBCFE-E326mad13B2βγ
cyclo -$CH_2CF_2CBrFCH_2$-O-	HBFE-CE353fbcB1

HALON NUMBERING SYSTEM

An alternate numbering system, the Halon Numbering System, is often used for fire extinguishing agents, particularly those containing bromine. This designation system is sometimes used for materials other than fire extinguishants. The Halon Numbering System designation lists, in order, the number of carbon, fluorine, chlorine, and bromine atoms in a molecule. NMERI/CGET has extended this convention to add a 5th number to designate the number of iodine atoms if needed. Trailing zeros are dropped. Thus Halon 1211 is $CBrClF_2$ and Halon 1301 is $CBrF_3$. The Halon Numbering System cannot specify isomers; both $CBrF_2CBrF_2$ and CF_3CBr_2F are designated Halon 2402. The Halon Numbering System is not used for cyclic or unsaturated compounds.

NMERI/CGET HALOCARB© COMPUTER PROGRAM

NMERI/CGET has developed a computer code written in BASIC language that determines the IUPAC name, Halocarbon Number, halon number, and molecular weight for

halocarbons from the structural formula. A copy of the compiled DOS program, HALOCARB.EXE©, is available on request.

To start the program, type "HALOCARB.EXE" from the A>, B>, or C> prompt depending on the drive containing the program. The program will then ask for a structural formula of the compound. The structural formula can be entered in any order and with any combination of capital and lower case letters. Numbers normally subscripted are entered as unsubscripted. A carbon atom must be entered first ("C" or "c") followed by the elements attached to that carbon atom. This process is repeated for each carbon atom. For example, the compound $CHClFCF_3$, HCFC-124, could be entered as "chclfcf3," "cf3cfclh," "cHcLfCf3," etc. For this example, the formula cannot be input as "C2HCLF4" (the structural formula rather than the empirical formula must be used) or as "CHCLFCFFF" (subscripts and not repeated letters must be used). If an impossible or unrecognized entry is given, the program will give an error message and will ask for a re-entry. The program will return the halon number, the Halocarbon Number (with the right isomer designation), the proper IUPAC name, and the molecular weight. Upon completion for one compound, the program asks for a new entry for another compound. At this point, a new structural formula can be entered or execution can be terminated by entering "Q." This program has been thoroughly checked out and is believed to be accurate. The present version will not handle unsaturated, cyclic, or branched-chain compounds. Nor will it give isomer designation for compounds containing four or more carbon atoms. These features are being added to a new version under development.

One word of caution is that the program will assign Halocarbon Numbers to any molecule with up to 9 carbon atoms. This will give a number corresponding to the appropriate refrigerant number in ASHRAE Standard 34 for propane, ethane, and methane halocarbon derivatives; however, for derivatives of pentane, hexane, and higher hydrocarbons, numbers are obtained that do not correspond to the refrigerant numbers in the ASHRAE Standard because refrigerant numbers above 400 have been reserved for materials that are not pure halocarbons (e.g., blends and inorganics). Halocarbon Numbers and refrigerant numbers are not always the same.

APPENDIX B

2.25-FT^2 JET FUEL FIRE TEST DATA.

TABLE B-1. 2.25-FT^2 HEPTANE FUEL FIRE TEST DATA.

Agent	Extinguishment quantitities, lb	Flow rates, lb/s	Extinguishment times, s
Halon 1211	0.31	0.12	2.59
Halon 1211	0.47	0.12	3.90
Halon 1211	0.40	0.14	2.84
Halon 1211	0.65	0.16	3.98
Halon 1211	0.37	0.17	2.16
Halon 1211	0.46	0.17	2.69
Halon 1211	0.55	0.17	3.20
Halon 1211	0.28	0.18	1.60
Halon 1211	0.35	0.18	1.97
Halon 1211	0.46	0.18	2.55
Halon 1211	0.46	0.18	2.50
Halon 1211	0.51	0.19	2.63
Halon 1211	0.53	0.19	2.76
Halon 1211	0.30	0.22	1.39
Halon 1211	0.40	0.22	1.86
Halon 1211	0.53	0.24	2.20
Halon 1211	0.48	0.27	1.80
Halon 1211	0.53	0.47	1.12
10% 1-Bromopropane/90% HFC-236fa	0.74	0.17	4.42
10% 1-Bromopropane/90% HFC-236fa	1.11	0.17	6.43
10% 1-Bromopropane/90% HFC-236fa	1.08	0.17	6.19
10% 1-Bromopropane/90% HFC-236fa	0.78	0.18	4.27
HFC-236fa	1.90	0.17	11.08
HFC-236fa	2.13	0.18	12.06
HFC-236fa	2.57	0.20	13.08
HFC-236fa	1.73	0.21	8.21

TABLE B-1. 2.25-FT^2 HEPTANE FUEL FIRE TEST DATA (CONCLUDED).

Agent	Extinguishment quantities, lb	Flow rates, lb/s	Extinguishment times, s
15% 1-Bromopropane/85% HFC-236fa	0.67	0.15	4.58
15% 1-Bromopropane/85% HFC-236fa	0.89	0.16	5.54
15% 1-Bromopropane/85% HFC-236fa	0.75	0.22	3.40
25% 1-Bromopropane/75% HFC-236fa	0.93	0.18	5.14
25% 1-Bromopropane/75% HFC-236fa	0.90	0.18	5.00
25% 1-Bromopropane/75% HFC-236fa	0.78	0.19	4.14
25% 1-Bromopropane/75% HFC-236fa	1.10	0.22	4.89
25% 1-Bromopropane/75% HFC-236fa	0.90	0.22	4.12
15% 1-Bromobutane/85% HFC-236fa	0.98	0.19	5.21
15% 1-Bromobutane/85% HFC-236fa	0.95	0.21	4.52
Perfluorohexane (C_6F_{14})	1.3	0.38	3.38
Perfluorohexane (C_6F_{14})	1.26	0.45	2.82
Perfluorohexane (C_6F_{14})	0.7	0.29	2.39
Perfluorohexane (C_6F_{14})	1.0	0.28	3.55
Perfluorohexane (C_6F_{14})	1.1	0.43	2.55
Perfluorohexane (C_6F_{14})	1.28	0.33	3.83
Perfluorohexane (C_6F_{14})	0.78	0.32	2.45
HFPE-1164X	1.22	0.49	2.42
HFPE-1164X	0.94	0.38	2.50
10% 1-bromopropane/90% HFPE-1164X	1.02	0.17	6.04
25% 1-bromopropane/75% HFPE-1164X	1.45	0.29	5.07
25% 1-bromopropane/75% HFPE-1164X	0.76	0.29	2.60
25% 1-bromopropane/75% HFPE-1164X	1.61	0.40	4.02

APPENDIX C

NOZZLE DESIGN AND FILL DENSITIES

A. NOZZLE DESIGN EQUATIONS

A critical element of the extinguisher is the nozzle, which affects two primary design criteria: agent flow rate and pattern. The following sections describe nozzle design equations and how they can be applied to achieve desired flow rates and discharge patterns.

The flow of a fluid through an orifice or nozzle derives from considerations of potential and kinetic energy and is given by:

$$v = \sqrt{2gh} = \sqrt{2P / \rho} \qquad [C\text{-}1]$$

where v = the fluid velocity of exit from the nozzle, g = the gravitational constant, and h = the pressure head. P = the fluid pressure at the nozzle inlet, and ρ is the fluid density.

For a perfect, non-friction flow, the volume of fluid flowing per unit time is given as:

$$Q = A\,v \qquad [C\text{-}2]$$

where Q is the flow in volume per second and A is the nozzle cross-sectional area.

For a real fluid, the total volume flow rate is modified by the addition of a discharge coefficient, C, to the equation. C depends on both the nozzle shape and the pressure of the fluid at the nozzle inlet. The flow equation then becomes:

$$Q = C\,A\,\sqrt{2P / \rho} \qquad [C\text{-}3]$$

C is frequently broken into two components—C_c, the coefficient of continuity and C_V, the coefficient of velocity such that:

$$C = C_c \times C_V \qquad [C\text{-}4]$$

Figure C-1 shows the discharge coefficients for several typical nozzle orifice configurations.

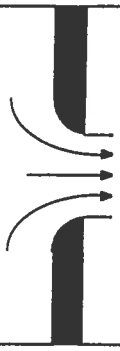
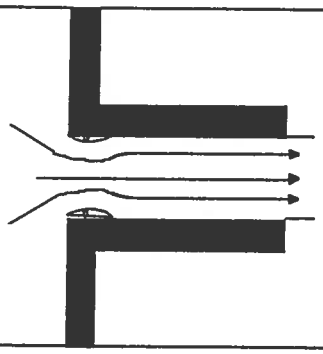
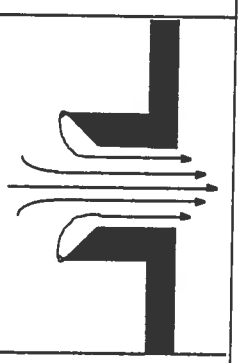
ORIFICES AND THEIR NORMAL COEFFICIENTS				
	SHARP EDGED	ROUNDED	SHORT TUBE	BORDA
				
C	0.61	0.98	0.80	0.51
C_c	0.62	1.00	1.00	0.52
C_v	0.98	0.98	0.80	0.98

Figure C-1. Discharge Coefficients for Several Typical Orifice Configurations.

The major fluid property missing from this simple equation is the fluid viscosity, μ. The effects of viscosity cause the flow of a real fluid to occur under two very different conditions or regimes, that is, laminar flow or turbulent flow. From experimental data, Reynolds (in 1883) deduced that the intermingling of fluid particles was absent at low fluid velocities and that the particles moved in parallel layers, or laminar flow, with no mixing. At higher velocities the fluid particles intermingled readily, i.e., they were in turbulent flow. Laminar flow would break down into turbulent flow at some critical velocity (the upper critical velocity) which was above the velocity at which turbulent flow would be restored to laminar flow (the lower critical velocity).

Reynolds generalized these conclusions by introducing a dimensionless parameter, N_R, later called the Reynolds Number, defined by:

$$N_R = v\, d\, \rho / \mu = v\, d / \nu \qquad [C\text{-}5]$$

where v = the fluid average velocity in the nozzle or pipe, d is the nozzle orifice diameter, ρ is the fluid density, μ is the fluid viscosity, and ν (the ratio of viscosity to density) is called the dynamic viscosity.

Certain critical values of N_R define the upper and lower critical velocities for all fluids in all pipes and nozzles. The upper limit for laminar flow lies in the range of N_R = 12,000 to 14,000. This number depends on the shape of the nozzle entrance, the roughness of the inner surface and the steadiness of the input pressure. These upper limits are of little practical interest in nozzle design.

The lower limit for turbulent flow is more important since it defines a condition below which all turbulence entering the flow from any source will be damped out by the viscosity, i.e., a limit below which laminar flow always occurs. This value of N_R is considered to be 2100.

N_R can be written in terms of nozzle pressure as follows:

$$N_R = (d \sqrt{2P / \rho}) / \nu \qquad [C\text{-}6]$$

For example, consider the following parameters used for the U.S. Army testing:

$d = 2.1$ mm

$\rho = 1.3$ g/cm^3

$P = 400$ lb$_f$/in^2 $= 2.76 \times 10^7$ dynes/cm^2

$\mu = 0.014$ poise $= 0.014$ dyne-s/cm^2

$\nu = 0.011$ cm^2/s

Thus N_R = 124,000 and the flow is turbulent.

Figure C-2 shows a calculated value for the discharge coefficient, C, as a function of Reynolds Number, N_R.

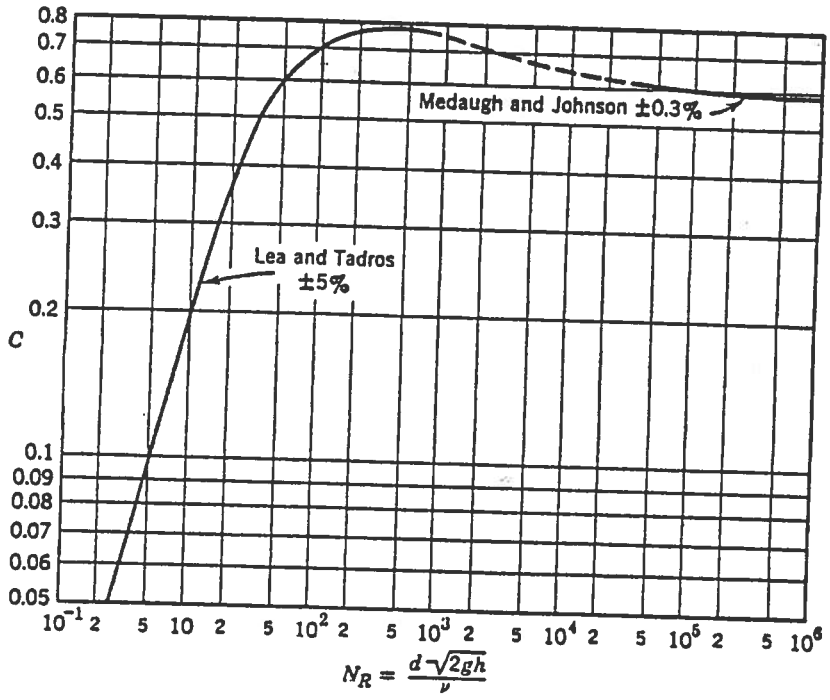


Figure C-2. Calculated value for discharge coefficient, C, as a function of Reynolds number, N_R. (Graphic developed from data in References C-1 through C-3).

From the equation C-3 for nozzle flow and considering the case for a sharp edged coefficient for the previous example:

$C = 0.61$ (from Figure C-1)

$A = 0.035\ cm^2$

$P = 2.76 \times 10^7\ dynes/cm^2$ (atmospheric pressure $= 1.013 \times 10^6\ dynes/cm^2$)

$\rho = 1.3\ g/cm^3$

Thus:

$$Q = 146\ cm^3/s = 190\ g/s = 0.42\ lb/s \qquad [C\text{-}7]$$

Therefore, a 4-lb charge should be discharged in approximately 9.6 seconds at an operating pressure of 400 lb_f/in^2.

Increasing the pressure to 600 lb_f/in^2 will increase the flow rate by a factor of $\sqrt{600/400}$ = 1.23; i.e., to about 0.52 lb_f/s and the 4-lb charge will be discharged in about 7.7 seconds.

On the other hand, a minor modification of the nozzle shape can change the flow rate by a factor of 0.98 / 0.61 = 1.61 via its effect on the discharge coefficient. The only modification required is to produce a rounded shape onto the inside edge of the nozzle orifice (Figure C-1).

The shape of the ejected material jet can be controlled or modified by converting the nozzle into a short channel instead of employing the simple orifice-in-a-wall configuration. For example, the use of a short tube (a length of the order of 3 times the diameter) will produce a much more highly directed stream of fluid while only reducing the rounded orifice discharge coefficient from 0.98 to 0.80. The tradeoff is that the "footprint" of the ejected fluid at the target is significantly reduced even as the range of delivery is increased.

For the purposes of this study, the effects of nozzle design on extinguisher discharge can be noted to have the following properties:

1. The discharge rate depends on the square root of driving pressure. Thus, doubling the driving pressure will produce a $\sqrt{2}$ = 1.4-fold increase in flow rate for a given nozzle.

2. For simple nozzles, the discharge coefficient can vary, at a given value of Reynolds Number, from a value of about 0.51 to 0.98 by simple variations of nozzle configuration for a given nozzle cross-sectional area. Thus, the flow rate can be most easily modified by changing the nozzle configuration.

3. The nozzle outflow pattern is most readily modified by changing the nozzle shape over a short distance from the nozzle orifice or point of constriction.

a) An outward bell-shaped nozzle produces a dispersed spray-like pattern with a large area coverage but which will not project the jet at large distances from the nozzle. The discharge coefficient of such a nozzle approaches 1.0.

b) A uniform tubular shape of the nozzle area over a dimension of several times the flow channel diameter will produce a strong jet that initially has the tubular shape of

the nozzle area, which will project to much larger distances than the spray-like pattern described above. The discharge coefficient of such a nozzle configuration usually approaches 0.80 - 0.85.

c) A nozzle having a gradual constriction toward its discharge end, particularly if an additional inner element is employed to produce two distinctly separate regions of flow across the nozzle area, will produce the longest jet throw distance. This is due to the formation of an inwardly directed sheath surrounding a slower moving core. Again, the real coverage of such a jet is smaller than either of the above configurations, and the nozzle constriction further reduces the flow by real considerations. The discharge coefficient of such a nozzle, aside from real considerations, approaches 0.5 - 0.6.

B. LIQUID FILL RATIOS

The liquid fill ratio of an extinguisher is the percent of the extinguisher volume occupied by the extinguishing agent in the liquid form. For example, if an extinguisher has an internal volume of 5 L (0.18 ft^3), a 75 percent fill ratio would require 3.75 L (0.13 ft^3) or [5 L (0.18 ft^3) x 0.75] of the liquid compound. The weight of the compound required will depend on the density of the compound. For example, a 75 percent liquid fill ratio of HFC-236fa is determined by multiplying the required volume of 3.75 L (0.13 ft^3) by the liquid density of HFC-236fa (1.37 g/mL at 25 °C [77 °F]). This results in 5.14 kg (11.3 lb) of HFC-236fa required to attain a 75 percent liquid fill ratio. The fill can also be expressed in terms of fill density. If we consider the same extinguisher with a volume of 5 L (0.18 ft^3) to be filled to a fill ratio of 75 percent, the fill density would be 5.14 kg divided by 5L, or after converting units, 1,028 kg/m^3 (64.2 lb/ft^3).

The importance of proper fill ratios cannot be overemphasized. High fill ratios cause flow rate problems, particularly toward the end of the discharge. High fill ratios leave less room for the nitrogen pressure charge, and as a result, the pressure drops off quickly during agent discharge, resulting in a rapid decrease in agent flow rate. A minimum flow rate must be sustained to achieve extinguishment. This problem is amplified when the extinguishers are cooled, since cooling a pressurized extinguisher to -45 °C can reduce the internal pressure by 100 lb_f/in^2 or more, depending on the initial pressure.

Another problem occurs when the extinguisher is heated. At high fill ratios (densities), the internal pressure rises rapidly as the temperature increases. For example, the internal pressure within an extinguisher of HFC-236fa having a fill ratio of 88.7 percent (equivalent to a fill density of 75.93 lb/ft^3) and initially charged with 360 lb$_f$/in^2 at 75 °F, will increase to approximately 900 lb$_f$/in^2 when heated to 60 °C (140 °F) (Figure C-3). This can cause higher than needed flow rates, which then decreases discharge times, and may result in a potential safety hazard if the extinguisher is not rated for the higher pressure. An understanding of fill ratios and fill densities is required to be properly fill extinguishers to achieve proper flow rates, spray patterns, and discharge times. Pressure versus temperature relationships at various fill densities for HFC-236fa are illustrated in Figure C-3.

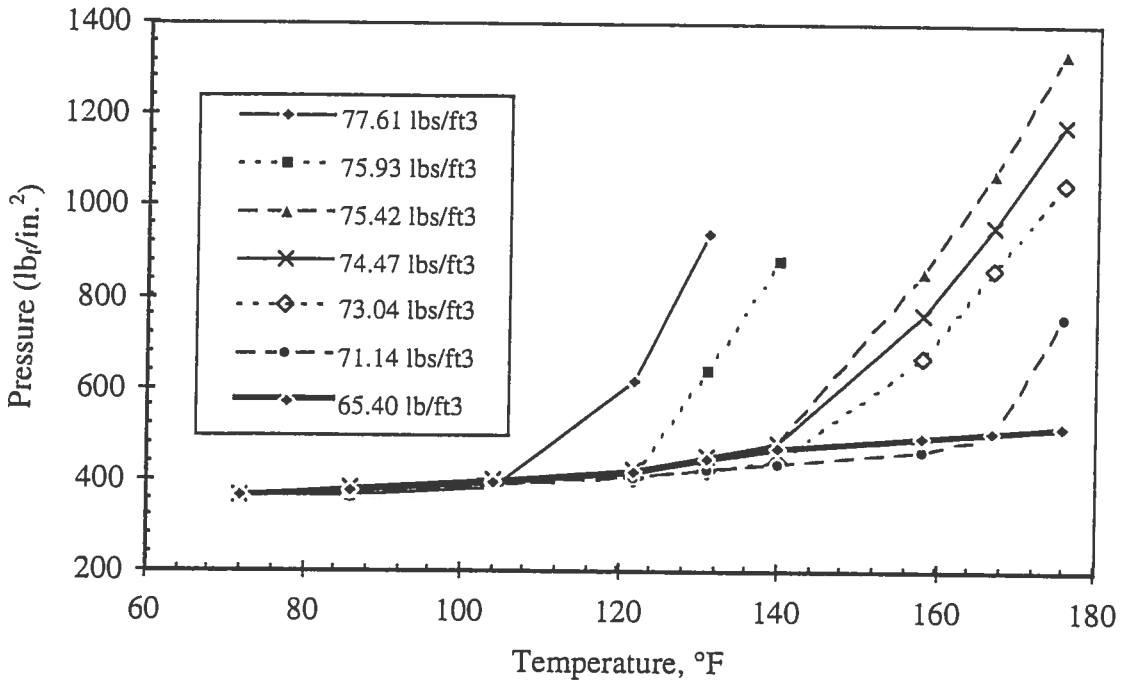


Figure C-3. Pressure Versus Temperature Relationships for HFC-236fa at Various Fill Densities (Reference C-4).

REFERENCES

C-1. Medaugh, F. W., and Johnson, G. W., *Civil Engineering*, Vol. 10, No. 7, p. 422, July 1940.

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C-3. Rouse, Hunter, and Howe, J. W., *Basic Mechanics of Fluids*, Wiley & Sons, New York, New York, 1953.

C-4. "NFPA 2001 Standard on Clean Agent Fire Extinguishing Systems 1996 Edition," National Fire Protection Association, 1 Batterymarch Park, Quincy, Massachusetts, February 1996.

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